

H2020-EINFRA-2015-1

VI-SEEM

VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean



Deliverable D5.3

User-oriented documentation and training material for VRE services

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Status –Version: Final – g

Date: September 30, 2017

Distribution - Type: Public

Abstract: Deliverable D5.3 – “User-oriented documentation and training material for VRE services” is the updated version of the documentation and training material for accessing, using and contributing to the VI-SEEM domain specific and generic services.

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The VI-SEEM project is funded by the European Commission under the Horizon 2020 e-Infrastructures grant agreement no. 675121.

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Document Revision History

| Date | Issue | Author/Editor/Contributor | Summary of main changes |
|-------------|--------------|--|--|
| 23-09-2016 | a | Michail Alvanos, Demetris Antoniadis | TOC |
| 17-10-2016 | b | Dusan Vudragovic, Vladimir Slavnic, Michail Alvanos, Constantinos Melachrinos, Panagiotis Charalambous, Demetris Antoniadis, Theo Christoudias, George Artopoulos, Zoe Cournia | 1 st draft |
| 26-10-2016 | c | Mihajlo Savic, Tamas Maray, Ioannis Liabotis, Anastas Mishev, Demetris Antoniadis | 2 nd draft |
| 29-10-2016 | d | Tamas Maray, Theo Christoudias, Ioannis Liabotis, Demetris Antoniadis | Comments to draft c, executive summary, introduction, conclusions, additions and corrections |
| 31-10-2016 | e | Demetris Antoniadis, Ognjen Prnjat, Ioannis Liabotis, Evangelia Athanasaki | Editing and corrections |
| 12-09-2017 | f | Andreas Athenodorou | 3 rd draft: Update according to reviewers' comments. |
| 30-09-2017 | g | Andreas Athenodorou, Ognjen Prnjat, Ioannis Liabotis, George Artopoulos, Theodoros Christoudias, Panayiotis Charalambous, Lidija Milosavljevic | Moved to new template, Comments to draft f, additions and corrections, quality control |

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References

- [1] Project VI-SEEM-675121 - Annex I - Description of the action
- [2] VI-SEEM D5.1 - Detailed technical implementation plan for VRE services and tools

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Glossary

| | |
|----------------|---|
| AMBER | Assisted Model Building with Energy Refinement molecular simulation programs |
| AFMM | Automated Frequency Matching Method |
| CBIR | Content-Based Image Retrieval |
| COSMO | Consortium for Small-scale Modeling |
| CPU | Central Processing Unit |
| CRYSTAL | Computational tool for solid state chemistry and physics |
| DICOM | Digital Imaging and Communications in Medicine |
| DREAM | The Dust REgional Atmosphere Model |
| ECHAM | Global Climate Model developed by the Max Planck Institute for Meteorology |
| EMAC | ECHAM/MESSy Atmospheric Chemistry |
| ERT | Electrical Resistivity Tomography |
| FERRET | Interactive computer visualization and analysis environment |
| FFTW | Fastest Fourier Transform in the West, library for computing the discrete Fourier transform |
| FIRFLY | Ab initio and density functional theory chemistry program |
| GAMESS | General Atomic and Molecular Electronic Structure System is a general ab initio quantum chemistry package |
| GATK | Genome Analysis Toolkit |
| GIS | Geographic Information System |
| GPU | Graphics Processing Unit |
| GPGPU | General Purpose Graphics Processing Unit |
| GrADS | Grid Analysis and Display System |
| GROMACS | Molecular Dynamics Software Toolkit |
| GUI | Graphical User Interface |
| HPC | High Performance Computing |
| IDL | Interactive Data Language, a programming language used for data analysis |
| LAS | Live Access Server |
| MEDICI | A multimedia content management system |
| MESSY | Modular Earth Sub-model System |
| MM5 | The PSU/NCAR mesoscale model |

| | |
|-----------------|---|
| NAMD | Scalable Molecular Dynamics Toolkit |
| NCL | NCAR Command Language |
| NetCDF | Network Common Data Form |
| NWCHEM | High Performance Computational Chemistry Software |
| OPENFOAM | Open source Field Operation And Manipulation toolbox for continuum Mechanics |
| PIDs | Persistent Identifiers |
| RegCM | The Regional Climate Model system |
| SEEM | South East Europe and Eastern Mediterranean region |
| SOL | Soft Ontology Layer |
| VI-SEEM | VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean |
| VRE | Virtual Research Environment |
| WEST | Wind Energy Simulation Toolkit |
| WRF | Weather Research and Forecasting Model |

Executive summary

What is the focus of this Deliverable?

The focus of this deliverable is to present the updated status of the VI-SEEM services documentation and training material available to the VI-SEEM target user communities. VI-SEEM provides documentation and training material both for the domain-specific services targeting the three scientific communities (Climate, Digital Cultural Heritage and Life Sciences) and for the VI-SEEM generic services, that is the e-Infrastructure services. Moreover, the deliverable presents documentation and training material for integrating new modules, workflows and datasets in the VI-SEEM services and adding new services to the VI-SEEM Virtual Research Environment.

This manuscript provides an update of the deliverable D5.3 incorporating the comments given by the reviewers as a result of the 1st periodic review. The main aim of this deliverable is to describe the improved access and presentation of the training material. A number of changes and updates have been made. The consortium has kept the high-level organization of the front page and at the same time reorganized each section in meaningful categories captured by different tabs. These categories were chosen according to practical criteria, depending on the scientific community, so that they provide more intuitive, quick and direct access to the relevant training material. These sub-sections are subsequently organized in different parts directing the user to the relevant training material. For instance section ["VI-SEEM applications"](#) in "Climate software and tools" is now organized in the three sub-sections: "Regional Climate Modelling", "Air Quality Modelling" and "Weather Forecast". In addition the portal was populated with more material. As an example all Application-level services such as Live Access Server, ChemBioServer, AFMM, Subtract, NANO-Crystal, DICOM Network and Clowder are accompanied with tutorials. Finally, in order to enhance the accessibility to the training material, a search machine is provided below the header of the training portal.

What is next in the process to deliver the VI-SEEM results?

The documentation and training material presented in this deliverable provides support to the development and integration of domain-specific services, tools, codes and datasets in the VRE platform, and general support to the users of the VRE platform. The material provided guides the applications selected for the Integration Phases, and the applications selected through the VI-SEEM Open Calls on how to integrate their results into the VRE platform and make them available to the Scientific Community. The results and conclusions from this deliverable are used by the following activities:

- WP2.3-Training
- WP4.2-Data access, preservation and re-use
- WP4.3-Data collection and provisioning
- WP4.4-Data analysis
- WP5.3-Development of the VRE platform
- WP5.4-Overall integration of services
- WP5.5-Scientific Support
- WP6.2-Implementation of open calls for access to VRE resources

- WP6.3-Integration of the new applications to the VRE environment

The complete description of the activities and inter-dependencies can be found in the VI-SEEM DoA [1].

What are the deliverable contents?

After a short introduction, an overview of the VI-SEEM domain-specific and generic services is provided. Next, the documentation and training material for the domain-specific services available through the VI-SEEM 1st, 2nd and 3rd integration phases is presented. Next, documentation on how to integrate software, workflows, data and additional services to the VI-SEEM VRE is provided. Finally, documentation and training material on the use of the e-Infrastructure services is listed.

Conclusions and recommendations

This deliverable lists the user-oriented documentation and training material for the VI-SEEM Virtual Research Environment services. The documentation and training material are used to provide scientific and technical support to the VI-SEEM user communities for using and extending the VRE services.

The deliverable takes into account the different user roles that can be taken by the VRE users and thus provides specific documentation depending on the aims of each user. For users of the domain-specific services interested in enhancing their research and education capabilities, the deliverable lists documentation and training material for the software, workflows, datasets and application-specific services available in the VRE environment. These services were made available through the 1st, 2nd and 3rd Integration phases. Additional material will be added as the 3rd integration phase progresses, as well as a result of the implementation of the VI-SEEM open calls. For users that want to contribute to the VRE, specific high-level guidelines are provided, listing all steps and material required for making their software, workflows and datasets available through the VRE environment. Finally, links to the documentation on the use of the VI-SEEM generic computation and storage services are provided.

1. Introduction

This deliverable lists the user-oriented documentation and training material for the VI-SEEM Virtual Research Environment (VRE) services. The documentation and training material is being used to provide scientific and technical support to the VI-SEEM user communities for using and extending the VRE services. The deliverable has been updated to reflect reviewers' recommendations after the first periodic review, tackling organization, visibility and ease of access of to training material and the portal.

The VI-SEEM VRE is composed of several types of services ranging from access to multiple types of e-Infrastructure services (computational, storage services and underlying resources), as well as software, data, workflow repositories and application specific services. WP5 oversees the integration of software tools, workflows, datasets and application-specific services to the VRE. As part of this it collects and lists, through the VRE portal, the available material that will assist the user communities of developing and integrating their application and use cases in the VRE.

End-users of these services can have multiple roles. In the case of the software, data, workflow repositories and applications specific services, the end-user can be either a user or a contributor of a new module or services, or both. In this deliverable we distinguish between these two different roles organizing the documentation and training material in different sections for each role.

For the user role we provide documentation on how one can use the software, data, workflows and application specific services for research and educational purposes. The deliverable provides the material made available through the 1st Integration Phase completed during month 12 of the project, the 2nd ended in month 18 and the 3rd which is expected to end on month 26. The documentation and training material provided by the use cases in these three integration phases is now available to the Scientific Communities in order to be able to use the tools and datasets made available. Furthermore, documentation and training material will be made available as the 3rd integration phase progress.

For the contributor role, the deliverable provides specific documentation on how interested researchers can make their software, workflows, datasets and application specific service available to the Scientific Communities through the VRE environment. Finally, we provide documentation for the use of the VI-SEEM generic services, i.e. e-Infrastructure services, available to both user categories.

The rest of the document is structured as follows: Section 2 provides the description, characterization and classification of the VI-SEEM services and resources that will assist the reader to understand the types of services offered. Emphasis is given to the structure of the training portal which is the main interface where training documentation is shared. Section 3 provides the available documentation and training material for the users of the VRE platform. It lists material collected through the VI-SEEM three Integration phases. This material will be further expanded as the 3rd integration phase progresses. Section 4 provides documentation and training

material for the VRE contributor. Section 5 provides documentation and training material for the generic services made available by WP3 and WP4. Finally Section 6 presents the conclusions and recommendations.

2. The VI-SEEM Virtual Research Environment

In this section we briefly list the available VI-SEEM services and their role in collecting the training material.

2.1. VI-SEEM application domain services

Through the analysis of the survey, conducted in December 2015 and presented in D5.1 [2], the services that the applications participating in the VI-SEEM Integration Phases offer to the three scientific communities were divided into 3 generic services and one service category that will contain domain-specific application services. Here we briefly mention the different services providing some information on what will be provided.

2.1.1. VI-SEEM scientific application environment

This service provides access and information to several modules such as optimized applications and libraries, VM images and list of codes, relevant to the work of the regional scientific communities of interest. In the following three tables we list the modules provided by the VI-SEEM community for each Scientific Community. More details can be found in D5.1 [2].

Climate

| | | | | |
|-----|----------|-------|----------|--------|
| WRF | WRF-CHEM | EMAC | Paraview | FERRET |
| NCL | DREAM | RegCM | GRADS | R |
| IDL | CCLM | GIS | OpenFOAM | MM5 |

Life Sciences

| | | | | |
|----------|----------|-----------|------------|--------------|
| NAMD | GROMACS | AMBER | Maestro | Desmond |
| VMD | Pymol | FFTW | R bbb | OpenCV |
| Rasmol | ImageJ | Vaa3D | GAMESS | FIREFLY |
| CRYSTAL | Molekel | Avogadro | siesta | Image-Pro |
| LabView | WinCoot | JVM | teseract | CellProfiler |
| PDB | TCL | Acml | apr | BioCORE |
| blacs | blender | Boost | cp2k | cuda |
| espresso | Gaussian | Hdf5 | ImageMagic | Lammps |
| maple | netcdf | Numactl | numpy | parallel |
| paraview | Phdf5 | Scalapack | scalasca | scipy |

Digital Cultural Heritage

| | | | | | |
|---------|-------|--------|--------|---------|-------|
| CLOWDER | 3DINV | ARCHES | AutoGR | CH-CBIR | IMC4H |
|---------|-------|--------|--------|---------|-------|

2.1.2. Workflow and software tools repository

This service provides access and information to several modules such as documents containing best practice procedures and workflows for the production of scientific results relevant to the application categories identified in the SEEM region. Examples of such documents are the workflows for simulating a protein with NAMD or with GROMACS (Life Sciences), and the MECCA atmospheric chemistry module on accelerator technology (Climate).

The Workflow and software tools repository service can be accessed on the "[Workflow, pipeline and software tools](#)" section of the VRE. This section provides access organized according to the scientific community. Namely it is split in a section dedicated to Climate, a section dedicated to Digital Cultural Heritage as well as a section on Digital Cultural Heritage. On the top of the page we provide three tabs which direct the user to the right part of the page. In the following three tables we provide the applications for which workflows and pipelines have been uploaded and those for which we expect material to be uploaded by the completion of the 3rd Integration phase (M26).

Climate

| Related Application | Description |
|--|--|
| <i>Applications for which workflows and pipelines have been uploaded</i> | |
| EMAC | MECCA atmospheric chemistry on accelerator technology. |
| VINE | Provides improved research in process-level understanding, considering the coupling and feedbacks: dust emission, dust ageing and dust deposition. |
| ClimStudyArmenia | Methods and methodologies for accurate weather prediction and climate change based on series of experiments. |
| ACIQLife | Methodology for performing reliable, comprehensive and detailed studies of the impact of lower atmosphere parameters and characteristics on the quality of life (QL) and health risks (HR) for the population. |
| TvRegCM | RegCM behavior for different model configurations. |
| <i>Applications for which workflows and pipelines are expected to be uploaded</i> | |
| Continuous_LTS | Continuous_LTS provides an algorithm used to fill gaps in satellite data which are caused due to cloud coverage. |

**Table 1. Workflows and pipelines for the Climate Scientific Community
Life Sciences**

| Related Application | Description |
|--|---|
| <i>Applications for which workflows and pipelines have been uploaded</i> | |
| MD-Sim | Workflows for simulating a protein with NAMD and GROMACS, Workflow for force field parameterization for ligand using AMBER force field and workflow for CADD with Glide. |
| CNCADD | Share scripts, tools and own codes |
| PSOMI | Workflow for the synthesis and spectroscopic synthesis of molecules. |
| CCC | Workflow for cancer cells classification. |
| THERMOGENOME | Workflow for measurement of thermodynamic stability of RNA/DNA and DNA/DNA duplexes. Perl and Python Software scripts for measurement of thermodynamic stability of RNA/DNA and DNA/DNA duplexes. |
| NGS1 | Documents with best practices and workflows for analysis of NGS data and list of pipelines using free libraries and software. |
| <i>Applications for which workflows and pipelines are expected to be uploaded</i> | |
| DICOMNetwork | Workflow for image exchange using different PACS technologies, based on DICOM (Digital Imaging and Communications in Medicine). |
| SQP-IRS | Workflows for protein sequence prediction VS. IR spectroscopic data Workflow for CADD for selected targets. |
| BioMoFS | Input files concerning GROMACS simulations of the double - stranded DNA hybridization |
| MDSMS | Analysis tools written in Tcl. |
| NGS2 | List of pipelines using free libraries and software for the discovery of mutations |

Table 2. Workflows and pipelines for the Life Sciences Community

Digital Cultural Heritage

| Related Application | Description |
|---|---|
| <i>Applications for which workflows and pipelines have been uploaded</i> | |
| VirMuf | Object digitization pipeline, Interactive 3D Museum tours, web UI, consultation services. |

| <i>Applications for which workflows and pipelines will be uploaded</i> | |
|---|---|
| Dioptra | Introductory level Semantic description of datasets documentation, meta-data definition, Reflectance Transformation imaging process description, structure from motion workflow. |
| | Real-time Immersive 3D Virtual Environment for Educational and Learning application development. |
| PETRA | The output can be provided as service and consultation. This includes: databank of surveyed materials, objects, facades, technical datasets of analyzed materials; consultation services of technical details and data analysis methodologies |

Table 3. Workflows and pipelines for the Digital Cultural Heritage Scientific Community

2.1.3. Regional community datasets

This service provides access and information regarding datasets of regional importance for the scientific communities of interest. Examples of such datasets are the Datasets with data for thermodynamic stability of RNA/DNA and DNA/DNA duplexes (Life Sciences). One can access the Regional Community datasets [online](#). At the bottom of the page there are three options corresponding to each scientific community:

2.1.3.1 Climate

Under the Climate Scientific Community tab, one is directed to the [page](#) which provides the user with links to the associated climate datasets in the VI-SEEM data repository (DSpace). The data sets are organized in four categories:

- Weather Datasets
- Analysis Datasets
- Air Quality Datasets
- Regional Climate Datasets

The Climate Scientific community provides access to the following datasets. Collections of these datasets will be constantly updated.

| Related Application | Description |
|--|--|
| <i>Applications for which datasets have been uploaded</i> | |
| WRF-ARW | Daily model output (raw output data as well as post-processed output). |
| VINE | Observation dataset on dust particles in ambient air |

| | |
|---|--|
| | available from Georgian National Environmental Agency. |
| RCM MENA-CORDEX | Gridded datasets of temperature and rainfall for the MENA, via the CORDEX data portals. |
| HIRECLIMS | ROCADA (Romanian Climatic Dataset). |
| WRF-Chem (NOA) | WRF-Chem dust aerosol concentrations and various meteorological parameters. |
| DREAMCLIMATE | Downscaled atmospheric-dust DREAM covering wide North Africa, Southern Europe and Middle East regions. |
| TVRegCM | Workflow for validation of RegCM using regional data. |
| ClimStudyArmenia | WRF Model Output for Severe Weather Forecasting over the territory of Armenia for June 2016. |
| <i>Applications for which datasets are expected to be uploaded</i> | |
| ACIQLife | Workflow for computing air quality indices |
| DRS-ACS | Characteristic constants describing the kinetics of atmospherically relevant processes and spectroscopic properties of the involved species. |

Table 4. Datasets for the Climate Scientific Community

2.1.3.2. Life Sciences

Under the Life Sciences tab, the user is directed to the [page](#) which provides the user links to associated Life Science datasets in the VI-SEEM data repository (DSpace). The data sets are organized in five categories:

- Modeling and Molecular Dynamics Datasets
- Computer aided Drug Design Datasets
- Analysis of Next Generation Sequencing Datasets
- Synchrotron Data Analysis Datasets
- Image Processing For Biological Applications Datasets
- Computational Simulation of DNA and RNA Datasets

In addition, datasets such as those of DICOMNetwork, which belong to the corresponding application-level service, can be accessed through the associated interface. For example, the [DICOM Network](#) provides access to investigations for medical staff with the appropriate access rights and as well as for patients to their personal radiography investigations. Currently, the system collects and processes more than 500 gigabytes of data per month.

The Life Science community is already providing and expected to provide access to the following datasets.

| Related Application | Description |
|---|--|
| <i>Applications for which datasets have been uploaded</i> | |
| MD-Sim | MD trajectories of oncogenic proteins with mutations relevant to the SEEM area. |
| DICOM Network | Generalized statistical datasets. Patient dataset available after special permission or relevant anonymization of data. |
| PSOMI | Datasets with molecule synthesis results. |
| <i>Applications for which datasets are expected to be uploaded</i> | |
| CNCADD | Produce and share parameter sets relevant to the community. |
| SQP-IRS | Biological dataset. Computational vs. Experimental database for proteins secondary structures. Crystallographic vs. Spectroscopic database for selected targeted proteins. |
| THERMOGENOME | Datasets with data for thermodynamic stability of RNA/DNA and DNA/DNA duplexes for all transcripts, exons, introns, 5-UTRs, 3-UTRs for Homo sapiens (human), A. thaliana, C. elegans, D. melanogaster, D. rerio. |

Table 5. Datasets for the Life Science Community

2.1.3.3. Digital Cultural Heritage

Under the Cultural Heritage Community tab, the user is directed to the [page](#) which provides to the user links to the associated Digital Cultural Heritage Datasets in the VI-SEEM Clowder platform. Clowder is the flagship application-level service of the Digital Cultural Heritage Scientific Community. Clowder is a research data management system designed to support any data format and multiple research domains. In addition when new data is added to the system, pre-processing is off-loaded to extraction services for extracting appropriate data and metadata. Users can upload, download, search, visualize and get various information about these data. Hence, it is useful to upload Digital Cultural Heritage Datasets in Clowder. The associated datasets are, therefore, stored in Clowder. Of course, the VI-SEEM data repository (DSpace) is also hosting these datasets. The Digital Cultural heritage datasets are organized in three categories:

- Pre-processed data
- Documentation and analysis datasets
- 3D Visualization and Analysis Data

The Digital Cultural Heritage Scientific community is already providing and expected to provide access to the following Datasets.

| Related Application | Description |
|---|--|
| <i>Applications for which datasets have been uploaded</i> | |
| ELKA | Karamanlidika texts |
| BVL | Banatica database: 1000 books and 200 digitized books |
| 3DINV | Existing and new datasets of geoelectrical tomographic data collected from field campaigns. |
| Manuscript | Datasets of digitized handwritten documents in Arabic or Hebrew. |
| CH-CBIR | Aerial images with annotated land cover types. Learned image representations for imagery in the areas of cultural heritage and remote sensing. |
| VirMuf | 3D models, CH Multimedia content and geo-spatial data. |
| PETRA | MEGA Jordan GPS/ geo-referenced data. |
| CSAD | Hundreds of RTi files of Ptolemaic inscriptions. |
| <i>Applications for which datasets are expected to be uploaded</i> | |
| AutoGR | A demo dataset will be used for demonstration purposes and shared with the VI-SEEM community for research purposes. |
| CHERE | Digital Libraries, Interactive Visualization Tools, Document Repository. |
| IMC4CH | Digital material for archaeological monuments. |
| Dioptra | Ontologies and RIVEEL3D |

Table 6. Datasets for the Digital Cultural Heritage Scientific Community

2.1.4. Application-level services for the regional communities

This category contains Web-based or visualization services providing easy access to underlying workflows, applications, and resources. Currently there are seven available Application-Level Services: one for Climate, five for Life Science and one for the Digital Cultural Heritage Scientific Communities. A description of these seven application-level services is provided below:

2.1.4.1. Climate

2.1.4.1.1. Live Access Server

The Live Access Server (LAS) is a highly configurable web server designed to provide flexible access to geo-referenced scientific data. It can present distributed data sets as a unified virtual data base through the use of DODS networking. The LAS uses the

Ferret visualization application by default, though other applications (Matlab, IDL, GrADS, etc.) can also be used. Functionality is added to be able to export to Google Earth.

LAS enables the web user to:

- visualize data with on-the-fly graphics
- request custom subsets of variables in a choice of file formats
- access background reference material about the data (metadata)
- compare (difference) variables from distributed locations

LAS enables the data provider to:

- unify access to multiple types of data in a single interface
- create thematic data servers from distributed data sources
- offer derived products on the fly
- remedy metadata inadequacies (poorly self-describing data)
- offer unique products (e.g. visualization styles specialized for the data)

The VI-SEEM LAS service is accessible on the web at <http://las.vi-seem.eu/>. The layout of the Live Access Server front page is shown in Figure 1. [Documentation](#) on how a researcher can use online the Live Access Server and install its Virtual Machine can be found on the VI-SEEM training portal.

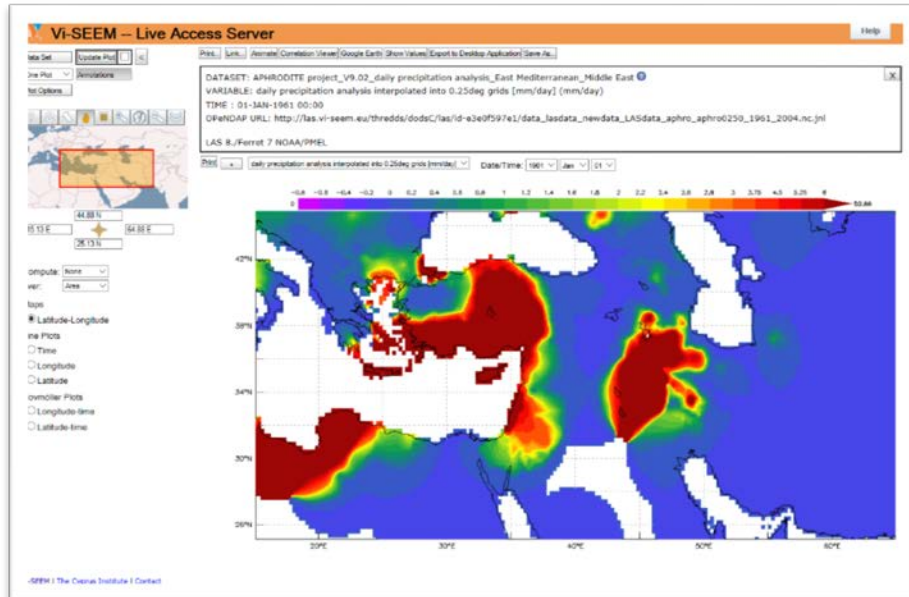


Figure 1. The Live Access Server front page

2.1.4.2. Life Sciences

2.1.4.2.1. **ChemBioServer**

ChemBioServer is a publicly available web application for effectively mining and filtering chemical compounds used in drug discovery. It provides researchers with the ability to:

- browse and visualize compounds along with their properties
- filter chemical compounds for a variety of properties such as steric clashes and toxicity
- apply perfect match substructure search
- cluster compounds according to their physicochemical properties providing representative compounds for each cluster
- build custom compound mining pipelines and
- quantify through property graphs the top ranking compounds in drug discovery procedures.

ChemBioServer allows for pre-processing of compounds prior to an in silico screen, as well as for post-processing of top-ranked molecules resulting from a docking exercise with the aim to increase the efficiency and the quality of compound selection that will pass to the experimental test phase.

Furthermore, successful applicants will get access to all public services, data sets, workflows and codes available in the VI-SEEM VRE Portal - <https://vre.vi-seem.eu>.

The number of accepted projects will depend on the technical and scientific merit of the proposals and the availability of resources. HPC projects are expected to be assigned a maximum of 3 Million core hours. A larger number of requested core hours will require elaborate and well documented justification.

The VI-SEEM ChemBioServer service is available online at <http://bioserver-3.bioacademy.gr/Bioserver/ChemBioServer/>. The layout of the ChemBioServer is shown in Figure 2. ChemBioServer Tutorials can be accessed through the training portal. There are two ChemBioServer tutorials available on the VI-SEEM training portal:

- <https://training.vi-seem.eu/images/trainingMaterial/LifeSciences/ChemBioServerTutorial1.pdf>
- <https://training.vi-seem.eu/images/trainingMaterial/LifeSciences/ChemBioServerTutorial2.pdf>

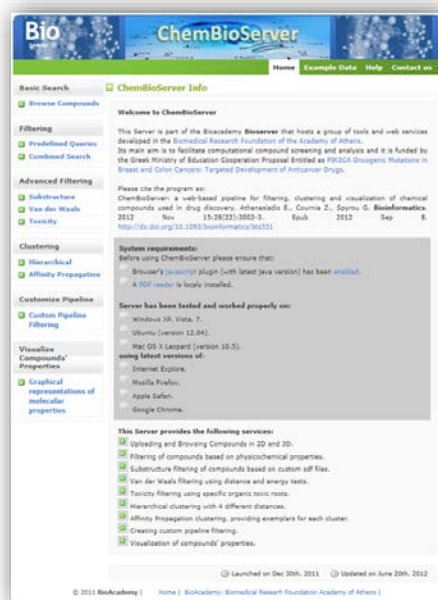


Figure 2 The ChemBioServer front page

2.1.4.2.2. AFMM

AFMM provides an automated platform with which the users can generate parameters for modeling small molecules with Molecular Dynamics simulations. The method used, fits the molecular mechanics potential function to both vibrational frequencies and eigenvector projections derived from quantum chemical calculations. The program optimizes an initial parameter set (either pre-existing or using chemically-reasonable estimation) by iteratively changing them until the optimal fit with the reference set is obtained. By implementing a Monte Carlo-like algorithm to vary the parameters, the tedious task of manual parameterization is replaced by an efficient automated procedure. The program is best suited for optimization of small rigid molecules in a well-defined energy minimum, for which the harmonic approximation to the energy surface is appropriate for describing the intra-molecular degrees of freedom.

Due to the abundance of organic molecules, no parameters have been created for the full chemical space. Thus, there is a great need for molecule parameterization before proceeding to Molecular Dynamics calculations. AFMM allows users to access parameters for their Molecular Dynamics simulation of small organic molecules that can be used as drugs or materials.

The VI-SEEM AFMM service is available [online](#). Documentation on the usage of AFMM is available [online](#) on the VI-SEEM training portal.

2.1.4.2.3. NANO-Crystal

NANO-Crystal is a web-based tool and has been implemented for the construction of spherical nanoparticles of a given radius.

More specifically, its goal is to find the number and the Cartesian coordinates of smaller spheres that fit on the surface of the nanoparticle and visualize the output morphology. The home page menu allows two selections for the user:

- (i) the radius of the nanosphere (nm), and
- (ii) the radius of smaller spheres (nm), that will cover the surface of the nanoparticle

The program computes the number of smaller spheres that fit on the bigger surface and the user can download their Cartesian coordinates (output format .xyz). The program code is implemented using PHP server-side scripting language, which is embedded into the HTML and CSS code. JQuery, a cross-platform JavaScript library, is also used. For local host of the webpage tool, the Wamp server is used. Moreover, the developers have developed a crystal computational morphology toolbox for constructing and modeling different crystal nanoparticle shapes. They use computational approaches for computing the macroscopic morphology of any periodic crystal by forming different shapes based on Miller indices and the distance measure from the center of the crystal and visualizing the resulting crystal. That crystal is a polyhedron that is created as the intersection of multiple polyhedra and individual planes via the steps that follows. This tool is planned to be imported in the NANO-Crystal webserver within 2017.

This tool enables users to construct spherical nanoparticles. Moreover, 2017 a new code under development will enable the user to construct different crystal nanoparticle shapes based on Miller indices and the distance measure from the center of the crystal.

The VI-SEEM NANO-Crystal application level service is available [online](#). A tutorial on NANO-crystal is available [online](#) on the VI-SEEM training portal.

2.1.4.2.4. Subtract

Subtract is an online tool that can calculate the volume of a binding site found in a protein. Subtract accepts an atom selection in the form of a PDB file and computes the three-dimensional convex hull of the atoms points with the help of SciPy library. The next step of the algorithm is to compute the volume of the convex hull and the volume of the atoms that are included in the solid based on their van der Waals radii. The subtraction of those two volumes yields the volume of the investigated cavity. The algorithm computes cavity volumes of trajectory frames in parallel for maximum efficiency and speed. It requires minimal usage of memory due to the fact that it follows a buffering strategy of reading file chunks and therefore there is no need to load the entire file into memory. There is a wide support of trajectory formats like Gromacs trajectory files and multi-model PDB files due to its dependency to the MDTraj library.

The measurements are evaluated for statistical significance using Wilcoxon Signed-Rank test and had their null hypothesis rejected (p -value < 0.005). Subtract is a tool that has been created to solve the problem of accurate measurement of the protein binding sites, and works both for crystal structures downloaded from the Protein Data

Bank and for protein structures arising from Molecular Dynamics simulations trajectories.

The VI-SEEM Subtract application level service is available [online](#). A tutorial on the Subtract can be accessed [online](#) through the VI-SEEM training portal.

2.1.4.2.5. DICOM

The “DICOM Network” provides access to investigations for medical staff with the appropriate access rights and as well as patients to the personal radiography investigations. Nowadays the system collects and processes more than 500 gigabytes of data per month. The system is based on Data Storage and Data Processing components distributed between different processing units and storages, which could be customized using specific interfaces. VISEEM integration connects the national DICOM Network application, which contains the existing DICOM Portal <http://dicom.md/>, with the DICOM Portal installed on VI-SEEM platform resources. DICOM DATA Interface grants the interconnectivity for different users of the both portals and allows displaying DICOM investigations using both portals interfaces. Public DICOM Server grants possibility for any VI-SEEM platform member to pull and retrieve the investigations from DICOM Network application and use the developed facilities based on configured access rules. VI-SEEM platform will offer possibility to install and configure publically available DICOM Portal that can be used by any interested institutions to store, access and share medical images. Setting up public DICOM Portal instance will increase the level of access to DICOM investigations and will help to promote DICOM Network services to regional medical research and practicing community.

The VI-SEEM DICOM Network application level service is currently [online](#). The DICOM Network front page is presented in Figure 3. A presentation on how one can use the DICOM Network can be found [online](#).



Figure 3. The DICOM Network front page

2.1.4.3. Cultural Heritage

2.1.4.3.1 Clowder

Clowder is a research data management system designed to support any data format and multiple research domains. It contains three major extension points: pre-processing, processing and previewing. When new data is added to the system, pre-processing is off-loaded to extraction services for extracting appropriate data and metadata. The extraction services attempt to extract information and run pre-processing steps based on the type of the data, for example to create previews. This raw metadata is presented to the user in the Clowder web interface. Users can upload, download, search, visualize and get various information about these data.

Data, in the case of VI-SEEM and more specifically in the field of Digital Cultural Heritage, can be of very diverse types and formats.

More specifically users can upload massively (zipped) or individual files of:

- 3D Models: where extractors clean up and prepare for visualization on the platform itself.
- Scanned books and their metadata: OCR algorithms will be used to extract the text in the documents so that users can find books using both metadata information and the book's contents.
- Image, text and sound files and their metadata, organized in collections.
- Advanced documentation data, such as Reflectance Transformation Imaging, and analysis of material properties of structures, works of art and artefacts.

The VI-SEEM Clowder service is currently located at <http://dchrepo.vi-seem.eu/>. The Clowder front page is presented in Figure 4 while functions such as Spaces and datasets access are shown in Figure 5 and Figure 6 respectively. A presentation on the usage of Clowder can be found [online](#) at the training portal.

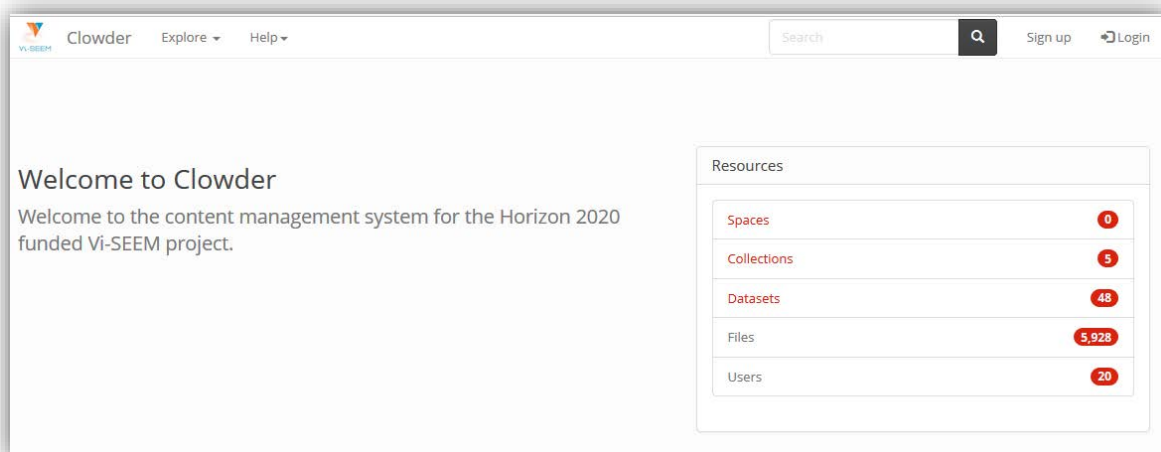


Figure 4. The VI-SEEM Clowder front page

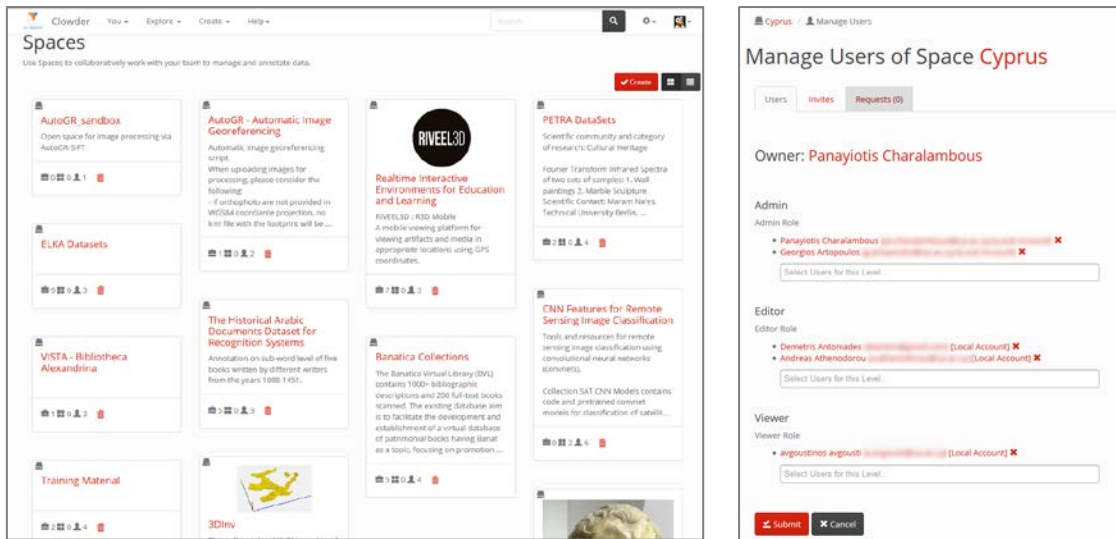


Figure 5. Spaces in the VI-SEEM clowder are used to organize datasets and the users that can access them

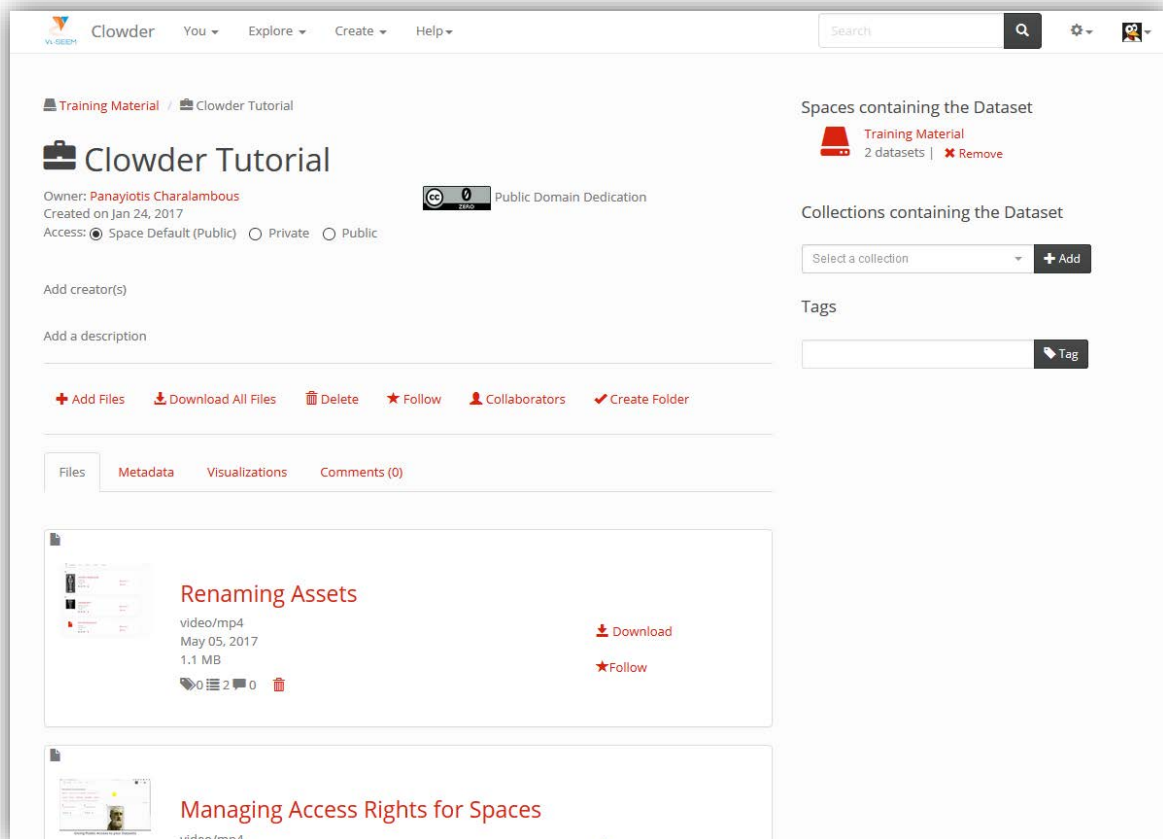


Figure 6. In the VI-SEEM Clowder, access and various properties of datasets can be set by owners

2.2. Tools for accessing VI-SEEM services and information

The following sections provide information on the VI-SEEM internal services that have been deployed and used in order to become the basic services that facilitate access to the user facing VI-SEEM services.

2.2.1. VI-SEEM VRE portal

The VRE portal provides access to the VRE services and applications. The portal connects the unified infrastructure developed in WP3, the generic data services deployed in WP4 and hosts the user-tailored front end interface. This integrated platform enables easy communication and data sharing between the various user groups. The VI-SEEM VRE portal is available at <http://vre.vi-seem.eu/>. The VRE portal is currently undergoing an update, following input from the first periodic review. The new layout of the portal will have an enhanced user-friendly character. The main section of the layout consists of sections specially designed for three classes of users:

- **Researchers:** From these parts of the webpage a Researcher could be directed to directions on how to:
 - Apply for Computational Resources
 - Access the Source Code Repository
 - Access to the supported applications & libraries
 - Access the Scientific Workflows
 - Access the Datasets
 - Access the training portal

- **Students:** From this part of the webpage a student could find directions on how to:
 - Access the Source Code Repository
 - Access to the supported applications & libraries
 - Access the Scientific Workflows
 - Access the Datasets
 - Access the training portal
 - Access to Upcoming Training Events

- **SMEs:** This section of the webpage is dedicated for SMEs, and provides all the necessary information to:
 - Apply for Computational Resources
 - Access the Datasets
 - Access the Use Cases

The updated version of the VRE portal is expected to be launched in the mid-October 2017.

2.2.2. VI-SEEM training portal

The VI-SEEM training portal collects and curates training material for the VI-SEEM services. Through the use of the training portal users have access to information for the available e-infrastructure services (HPC, Grid, Cloud and Data) as well domain specific material for using the tools and data provided. The VI-SEEM training portal is available at <http://training.vi-seem.eu/>.

The VI-SEEM training portal is the main source of the training material for the VI-SEEM users and it offers a number of important features which make the portal user friendly. The training-portal has a new enhanced user oriented character, which provides easy access to researchers, students and users in general.

The front page of the training portal consists of a header which provides access to the following training Material:

- Domain Specific Software and Tools
- Data and Visualization
- Common Computing Resources
- Event Related Training Material

In addition the header of the training portal provides a search engine.

The front page of the training portal, shown in Figure 7, has a high-level organization structured in three main categories:

- **Domain Specific Software and Tools** providing access to training material for
 - Climate Software and Tools
 - Digital Cultural Heritage Software and tools
 - Life Science Software and Tools
- **Data and Visualization** providing access to training material for:
 - Data
 - Storage Services
 - Visualization
- **Common Computing Resources** providing access to training material for
 - Cloud
 - High Performance Computers
 - Grid

Therefore, the training portal is organized in nine sections each one described by a distinct icon. By clicking on the icon the user is directed to the associated training material. In the next subsections we provide a description on the structure of each one of the nine sections.

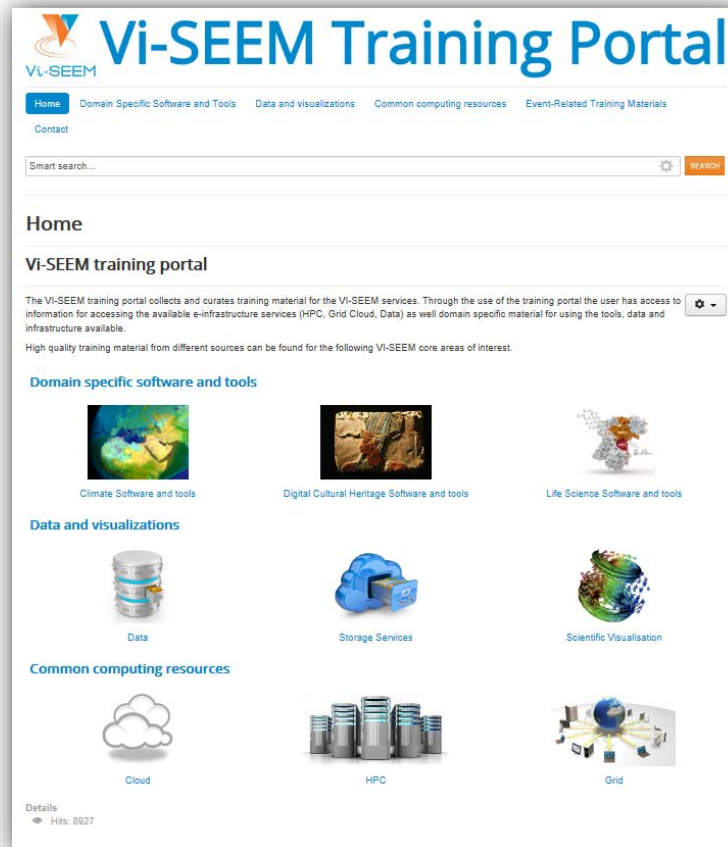


Figure 7. The front page of the Training Portal

2.2.2.1. Climate Software and Tools

From this webpage the user can access all the training material which is related to the VI-SEEM Climate applications as well as training material which is related to general software applications, modules and data structures used by the Climate Scientific Community. The structure of the webpage follows the needs of the Climate researchers within the VI-SEEM Project. Hence, the layout of the webpage is organized in five sections (tabs). These sections are the following:

- Live Access Server
- VI-SEEM Applications
- Visualization
- Software and tools
- General Training Material

The first tab provides access to the training material on the Live Access Server. The Live Access Server is the Application Level Service of the Climate Scientific Community; it is a web server providing flexible access to geo-referenced scientific data, offering visualization & post-processing capabilities for climate data.

The page also provides access to training material on the Climate applications which have been integrated in the VRE during the three integration phases. The associated

training material is organized in three sections. These sections are chosen to reflect the Climate Research areas supported by VI-SEEM:

- Regional Climate Modelling
- Air Quality
- Weather Forecast

An important tool which enables Climate Scientists demonstrating their results effectively is Visualization applications for climate. Therefore, a section of the training material is dedicated on Visualization. The next section focusses in Software and tools; namely it provides training material on the WRF and RegCM software as well as on NetCDF data format. Finally, more general training material is provided.

2.2.2.2. Digital Cultural Heritage Software and tools

From this webpage a user interested in VI-SEEM Digital Cultural Heritage applications can find the corresponding training material. The structure of the page has been designed in such a way so that it enhances its efficiency and reduces the time a user needs to seek for training material. Since the Digital Cultural Heritage community has a strong application-driven character, the webpage is organized in the following seven tabs named after the particular application and action:

- Clowder
- Vi-SEEM applications
- Content Management Systems
- Metadata
- Digitization
- Visualization
- General Training Material

The first tab provides access to training material on the Clowder. Clowder is the Flagship application of the Digital Cultural Heritage Scientific Community. Through the Clowder a user can access all DCH Datasets, and use all the associated visualization, digitization and other services. Thus, it comes first.

Subsequently VI-SEEM provides access to the training material related to the VI-SEEM applications developed in the three integration phases. The corresponding training material is organized in the following three sections:

- Digital Libraries
- Machine Learning for Digital Cultural Heritage
- Online Visualization Tools

The Remaining five tabs provide access to training material related to Content Management Systems, Metadata, Digitization, Visualization and General Training Material.

2.2.2.3. Life Science Software and Tools

A user can find all the training material related to the Life Sciences applications supported by VI-SEEM. The structure of this page has been tailored to the needs of the Life Scientific Community. It is organized in four tabs named after the corresponding research area:

Molecular Dynamics Simulations

- Computer Aided Drug Design
- Next Generation Sequencing Data Analysis
- Medical Image Processing

Each one of this tabs is subsequently organized in three distinct sections:

- General Training Material: This involves training material related to the application modules used in the particular research area.
- VI-SEEM applications: This includes training material related to the developed VI-SEEM Life applications.
- Application Level Services: This consists of the material, mostly tutorials, on how a user can use the particular Application-Level Service. For instance there the user can find tutorials and presentations on the usage of ChemBioServer, AFMM, Nano-Crystal, Subtract and DICOM Network.

2.2.2.4. Data

Data related training material can also be [accessed](#). The structure of this page has been tailored according to the relation of the Scientific Communities with their data consideration. It is organized in three tabs:

- General Training Material
- Climate
- Digital Cultural Heritage

A detailed description on the training material a user can find in this page, is provided in Section 5.3 of this manuscript.

2.2.2.5. Storage Service

Training Material related to Storage Services is available [here](#). We provide training material dedicated to the VI-SEEM Data Repository.

2.2.2.6. Scientific Visualisation

This page provides material for training purposes on [Scientific Visualization](#). This page is organized in three sections-tabs. This structure is in accordance with the cross-disciplinary character of VI-SEEM, thus we provide General Training Material which can be used by all three Scientific Communities. In addition we include Visualization Topics focusing on the scientific communities of Climate and Cultural Heritage. Thus, the tabs appearing in the webpage are the following:

- General Training Material
- Climate
- Digital Cultural Heritage

A detailed description on the training material which can be found in this page, is provided in Section 3.5 of this manuscript.

2.2.2.7. Cloud

Training Material focusing on Cloud computing can be obtained [here](#). The page is self-contained and is not organized in tabs. A detailed description of the provided training material can be found in Section 5.1.2.

2.2.2.8. HPC

Training material on High Performance Computers (HPCs) can be accessed [here](#). The above webpage provides the user with four options manifested by four distinct buttons:

- Practical HPC
- Development
- Improvement
- Applications

"Practical HPC" provides all the documentation and training needed to access and run a supercomputer. This part of HPC training consists of four different sections/tabs:

- Super Computer Basics
- Scripting
- Version Control
- Parallel Tools Platform

"Development" provides all the information one needs to know in order to develop an application capable to run on computers making use of multi-core architectures. The training material on Development is provided in six tabs:

- Programming
- Python
- OpenMP
- MPI
- GPU Programming
- General Training Material

"Improvement" provides documentation on topics which enable the user to analyze the performance of codes as well as to improve the codes and debug them. Optimizing a code running on HPCs is an important task which reduces the execution time and makes the runs less expensive in terms of power consumption. This part of the HPCs' training material splits in two tabs:

- Performance Analysis
- Code Improvement and Debugging

Finally "Applications" provide a number of cross-disciplinary documentations focusing on particular applications which make use of HPCs. Such applications are Synchrotron software and imaging software running on multicore architectures. A more detailed description of the training material on HPCs is provided in Section 5.1.1.

2.2.2.9. GRID

Training material focusing on GRID computing can be accessed [here](#). The page provides sliders with links to training material on several aspects of Grid computing. A detailed description of the associated training material can be found in Section 5.1.3.

2.2.3. VI-SEEM wiki

The VI-SEEM wiki aims to support site managers for operating the integrated VRE services on top of the underlying infrastructures. It contains information about the available services, the procedures for integrating existing services with the VI-SEEM e-infrastructure and how-to material for establishing new services and integrating them with the existing VRE services. The VI-SEEM wiki is available at <http://wiki.vi-seem.eu/>.

2.2.4. VI-SEEM service catalogue/portfolio

Service orientation of the e-Infrastructure projects is one of the major factors to their increased usability and extended sustainability. An important aspect of the service orientation is the IT service management. Following the FitSM standard, one of the most commonly used standards for IT service management, the first requirement for implementing the service management system is service portfolio management. To address this important requirement, an IT service catalogue and portfolio management system was developed for the needs of the VI-SEEM project. Maintaining the service catalog/portfolio current will result in better service visibility and higher infrastructure utilization.

The VI-SEEM catalog/portfolio management system currently allows two different data entry procedures: via the RESTful API or via the temporary service administration tool (SPMT WRITE DJANGO UI). The third way to enter data will be the write UI, which is in the final phase of the development. In this text, the data entry through the temporary service administration tool will be described.

SPMT implements the service portfolio and catalogue that has been described in VI-SEEM D3.2: "Service registry, operational and service level monitoring".

The SPMT READ user interfaces are available under the following links:

The Service Catalogue View UI: <https://services.vi-seem.eu/ui/catalogue/services/>

The Service Portfolio View UI: https://services.vi-seem.eu/ui/catalogue/services/#VI-SEEM_Service_Portfolio_Management_System

The Service Administration interface (SMPT WRITE UI) can be accessed via https://services.vi-seem.eu/ui/catalogue/services/#VI-SEEM_Login.

The Content of the VI-SEEM Service Catalogue as this appears in the corresponding webpage is presented in Figure 8.

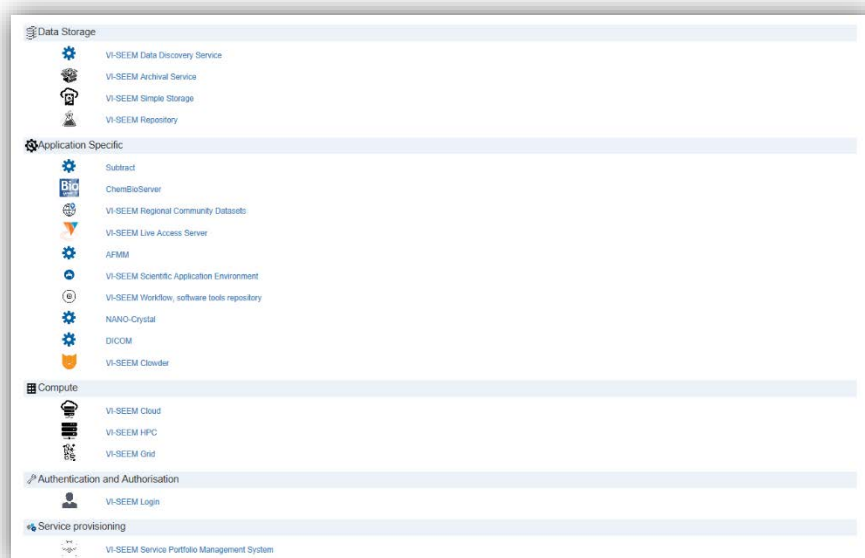


Figure 8. The content of the Service Catalogue as this is presented in the <https://services.vi-seem.eu> webpage

2.2.5. Code repository

VI-SEEM Code repository hosts tools, software and workflows made available from the VI-SEEM Scientific Application environment. It is deployed on top of the git open source system. GitLab is used to provide a usable web-based UI for project management and repository control. The service is fully integrated with VI-SEEM Login service, and it is available at <https://code.vi-seem.eu/>.

2.2.6. VI-SEEM repository

The VI-SEEM Repository provides long-term data preservation, suitable for data set sharing. VI-SEEM repository is based on DSpace. DSpace is an open source repository software package typically used for creating open access repositories for scholarly and/or published digital content. DSpace shares some features with content management systems and document management systems. In addition the DSpace repository software serves a specific need as a digital archives system, focused on the long-term storage, access and preservation of digital content.

The repository can be used for a variety of use cases like: (i) storage of curated data sets for longer term preservation, (ii) sharing those datasets with selected collaborators or opening them up to entire communities, via a web interface (iii) making such data sets searchable by means of associating meta data and then harvesting them and finally (iv) enabling scientific communities to capture and

describe digital works using a custom submission workflow module. The VI-SEEM Repository is available at <https://repo.vi-seem.eu/>.

2.2.7. Support ticket system

The support ticket system is available at <https://support.vi-seem.eu/> and represents an oSTicket installation hosted at UNI BL. Agent login is located at <https://support.vi-seem.eu/scp> and is to be used by support personnel of the project. Help topics currently include generic topics (feedback and reporting a problem) as well as VI-SEEM specific topic including: Infrastructure, Service Registry, Data Platform, Applications and Domain Specific Services.

2.3. Generic VI-SEEM VRE services

WP3 and WP4 provide generic infrastructure services for the VI-SEEM community. WP3 provides the unified underlying e-Infrastructure layer for the benefit of the Scientific Communities. WP4 deals with data lifecycle support for Scientific Communities including data sharing and reusability (comfortable way for effective collaboration), data archiving, data manipulation, collaborative access, common interfaces to storage, data annotation and citation, metadata, etc. Below we list the available generic services provided by the VI-SEEM VRE.

2.3.1. e-Infrastructure services

Within WP3 the following generic VRE services are provided:

VI-SEEM HPC (High Performance Computing) service allows users to perform complex simulations on the state-of-the-art computing hardware. The service delivers 18.8 CPU, 371.6 GPU, 16.0 Xeon Phi, and 5.3 IBM Cell millions of hours per year. It provides access to clusters with low-latency interconnection or supercomputers. Most of them are based on CPUs with x86_64 instruction set and equipped with accelerator cards, BlueGene/P systems are also available, as well as one based on the Cell processors. The access procedure is described on the VI-SEEM [wiki](#).

The VI-SEEM Cloud service allows users to deploy on demand VM instances with custom services. This service provides the ability to launch VMs (Virtual Machines) with public/private IPs, and the possibility to deploy VRE (Virtual Research Environment) services for their production or backup/fail-over instances. In total 500 VMs or 4 million of VM-hours per year are made available for VRCs (Virtual Research Communities). Access procedure is described on the VI-SEEM [wiki](#).

VI-SEEM Grid service provides access to smaller, geographically distributed clusters integrated via Grid middleware. Access procedure is described on the VI-SEEM [wiki](#).

The VI-SEEM Login service enables research communities to access VI-SEEM e-Infrastructure resources in a user-friendly and secure way. More specifically, the VI-SEEM Login allows researchers whose home organizations participate in one of the eduGAIN federations to access the VI-SEEM infrastructure and services using the

same credentials they are using at their home organization. Furthermore, VI-SEEM Login supports user authentication with social identities, enabling even those users who do not have a federated account at a home organization to be able to seamlessly access the VI-SEEM services without compromising the security of the VI-SEEM infrastructure.

2.3.2. VI-SEEM data services

WP4 provides a generic data services portfolio for the benefit of the VI-SEEM community. Specific data services deployed are:

- VI-SEEM simple storage service (VSS)
- VI-SEEM repository service (VRS)
- VI-SEEM archival service (VAS)
- VI-SEEM work storage space / local storage and data staging (VLS)
- VI-SEEM data discovery service (VDDS)
- VI-SEEM data analysis service (VDAS)

From the user's point of view, four of these services (VSS, VRS, VAS and VLS) are more related to storage and two of them (VDDS and VDAS) are more related to data. Storage related services handle tasks from the start of the data lifecycle (VSS for storing/sharing data in its volatile phase) through the publication / reuse period (VRS for hosting/sharing data; VLS for work storage space and staging) to the long term preservation stage (VAS for archiving and safe data replication). Data related services on the other hand are more focused on the data (and its metadata) itself providing data discovery / flexible searching (VDDS) and distributed data analysis capabilities (VDAS). In addition to providing these assets for the VI-SEEM community, training materials are also being developed to help the users of VI-SEEM to take advantage of the generic data services portfolio.

All currently available VI-SEEM services are listed in VI-SEEM Service Catalogue (<https://services.vi-seem.eu/ui/catalogue/services/>).

3. User documentation and training material for the user communities

VI-SEEM carries on the integration of the top level-domain-specific services and applications into the e-Infrastructure and data service platforms of WP3 and WP4. The implementation plan for the development and integration of domain-specific services for the three scientific communities was set by D5.1 "Detailed technical implementation plan for VRE services and tools" [2]. During the writing of this deliverable the 3rd integration phase is running and material for each of services available for the scientific user communities is being constantly collected. In this section we list the user documentation and training material available to the user communities mainly through the 1st and 2nd integration phases. The user documentation and training material will be populated and updated as the integration phase continues to progress. Existing material are uploaded to the VI-SEEM training portal and linked through the VI-SEEM VRE Portal, while as new material is being prepared these will be also made available to users via the training and VRE portals.

3.1. VI-SEEM scientific application environment

Below we list the documentation and training material available for each scientific community in regards to the VI-SEEM scientific application environment. The material concerns optimized applications and libraries developed and used through the integration phases as well as scientific community specific use cases build upon the above modules.

3.1.1. Climate scientific community

The Climate Scientific Community currently provides the following training material:

| Medina Source-to-source KPP/EMAC to CUDA Pre-Processor | |
|---|---|
| Description | Directions on how to install and run the MECCA Fortran to CUDA |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#echam-messy-global-chemistry-climate-model-emas |

| VINE: VIAM/NEA Regional Chemistry-Climate Model | |
|--|---|
| Description | Tools (ncl, ncview) and software for the manipulation and visualization of the model's output as well as directions on how to set up and run the WRF (the meteorological driver) model and the WRF-Chem model over the south Caucasus domain. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#viam-nea-regional- |

| | |
|--|--|
| | chemistry-climate-model-vine |
|--|--|

| Tuning and Validation of the RegCM | |
|---|---|
| Description | Description and directions on how to install and run RegCM |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#tuning-and-validation-of-the-regcm-tvregcm |

| ClimStudyArmenia: Accurate Prediction and Investigation of Weather and Climate in Armenia and South Caucasus (WRF) | |
|---|---|
| Description | Training Material on SLURM and WRF model used in ClimStudyArmenia |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#accurate-prediction-and-investigation-of-weather-and-climate-in-armenia-and-south-caucasus-wrf-climstudyarmenia |

| WRF-Chem: WRF-Chem Regional Climate Modelling | |
|--|---|
| Description | Access to the webpage of the WRF-Chem where you can find, user documents, online tutorials etc |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#wrf-chem-regional-climate-modelling-wrf-chem |

| WRF-ARW: Operational Weather Research and Forecast Model | |
|---|---|
| Description | User's Guides for the Advanced Research WRF (ARW) Modeling System, and an online tutorial for WRF-ARW |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#operational-weather-research-and-forecast-model-wrf-arw |

| NCAR graphics user page | |
|--------------------------------|---|
| Description | NCAR Graphics is a Fortran and C based software package for scientific visualization |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#ncar-graphics |

| NCL user page | |
|----------------------|---|
| Description | NCL is an interpreted language designed specifically for scientific data analysis and visualization |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#ncar-command-language-ncl |

| WRF model user page | |
|----------------------------|---|
| Description | Users' page for the Weather Research and Forecasting Model |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#weather-research-and-forecasting-model-wrf |

| WRF-CHEM model user page | |
|---------------------------------|---|
| Description | Assist the users of WRF-Chem in the atmospheric chemistry community to compile and run WRF-Chem simulations |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#weather-research-and-forecasting-model-wrf |

| WRF-CHEM Advanced Research Modeling System Guide | |
|---|---|
| Description | The user's guides for the advanced research WRF (ARW) Modeling System, Version 3 |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#weather-research-and-forecasting-model-wrf |

| Tools and software for the manipulation and visualization of WRF-CHEM output | |
|---|---|
| Description | Material related to manipulation & visualization of WRF-CHEM output |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#tools-and-software-for-the-manipulation-and-visualization-of-wrf-chem-output |

| Regional Model: REGCM4: RegCM4 model code, installation and run | |
|--|---|
| Description | Setup and run WRF-CHEM model over the south Caucasus domain |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#regional-model-regcm4 |

| Main drivers for long-range climate prediction | |
|---|---|
| Description | Long-range climate prediction material |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#main-drivers-for-long-range-climate-prediction |

3.1.2. Digital Cultural Heritage scientific community

The Digital Cultural Heritage Scientific Community currently provides the following training material:

| Digital Humanities Course Registry | |
|---|---|
| Description | The Digital Humanities Course Registry is an inventory of Digital Humanities courses and programmes. It helps students, researchers, lecturers and institutions to find, add and connect them. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#digital-humanities-course-registry |

| Landscape services | |
|---------------------------|---|
| Description | A set of responsive web services that include large terrain datasets generation, 3D landscape composing and 3D model processing, leveraging on powerful open-source frameworks and toolkits such as GDAL, OSGjs, OpenSceneGraph and ownCloud. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#landscape-services |

| Technical Guidelines for Digital Cultural Content Creation Programmes | |
|--|---|
| Description | This document is intended as a resource for policy-makers, for those implementing funding programmes for the creation of digital cultural content and for those managing digitization projects. Based on a lifecycle approach to the digitization process, it seeks to provide guidelines for the use of technical standards and identifies areas where there is already a commonality of approach. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#technical-guidelines-for-digital-cultural-content-creation-programmes |

| Good Practice Handbook | |
|-------------------------------|---|
| Description | A list of good practices in digitization. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#good-practice-handbook |

| Digitization: standards landscape for European museums, archives, libraries | |
|--|---|
| Description | An overview of the different standards used from museums, libraries and archives, as well as ministries |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#digitization-standards-landscape-for-european-museums-archives-libraries |

3.1.3. Life Sciences scientific community

The Life Sciences Scientific Community currently provides the following training material:

| Principles of Computer-Aided Drug Design | |
|---|---|
| Description | Introduction on the principles and implementation of computer aided drug design. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#principles-of-computer-aided-drug-design |

3.2. Workflow, pipeline and software tools

Below we list the training material available for each scientific community in regards to the VI-SEEM workflow, pipeline and software tools service. The material concerns several modules such as documents containing best practice procedures and workflows for the production of scientific results relevant to the application categories identified in the SEEM region.

3.2.1. Climate scientific community

The Climate Scientific Community currently provides the following training material:

| Tuning and Validation of the RegCM | |
|---|---|
| Description | Installation, structure and main steps to run the model RegCM4 |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#tuning-and-validation-of-the-regcm-tvregcm |

| ClimStudyArmenia: Accurate Prediction and Investigation of Weather and Climate in Armenia and South Caucasus (WRF) | |
|---|---|
| Description | Installation Workflows, WRF as well as SLURM tutorials |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#accurate-prediction-and-investigation-of-weather-and-climate-in-armenia-and-south-caucasus-wrf-climstudyarmenia |

| Continuous land surface Temperature: Continuous_LTS | |
|--|---|
| Description | Training Material on Google Earth Engine |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#continuous-land-surface-temperature-continuous_Its |

| ACIQLife: Atmospheric Composition Impact on Quality of Life and Human Health (WRF/CMAQ) | |
|--|---|
| Description | A description of the ACIQ Life Code – Workflow |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#atmospheric-composition-impact-on-quality-of-life-and-human-health-wrf-cmaq-aciqlife |

| DRS-ACS: Dynamics, reactivity and spectroscopy of atmospheric chemical species | |
|---|---|
| Description | Training material on the DRS-ACS application with the corresponding FORTRAN code. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#dynamics-reactivity-and-spectroscopy-of-atmospheric-chemical-species-drs-acs |

| HIRECLIMS: High Resolution Climate Services for Southern Europe using regional climate modelling | |
|---|---|
| Description | Information on how to install, compile and run the CCLM (COSMO model in Climate Mode) as well as a description of the non-hydrostatic regional COSMO-Model (COSMO (Consortium for Small scale MOdeling)) |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#high-resolution-climate-services-for-southern-europe-using-regional-climate-modelling-cosmo-hireclims |

| OPENFoam: Wind simulation over rugged terrain | |
|--|---|
| Description | Tutorial on OpenFOAM Wind Simulation |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#wind-simulation-over-rugged-terrain-openfoam |

| WRF Installation workflow | |
|----------------------------------|---|
| Description | Workflow demonstrating Installation of WRF model |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#weather-research-and-forecasting-model-wrf |

| WRF check output and Troubleshooting workflow | |
|--|---|
| Description | The workflow for WRF check output and troubleshooting |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#weather-research-and-forecasting-model-wrf |

| VisTrails Training workflow | |
|------------------------------------|---|
| Description | VisTrails is an open-source scientific workflow and provenance management system that supports data exploration and visualization. The training material provides access to the VisTrails Wiki and an example of a VisTrails Workflow. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#vistrails |

3.2.2. Digital Cultural Heritage scientific community

The Digital Cultural Heritage Scientific Community currently provides the following training material:

| Manuscript demo: Historical Document Line Detection Using Neural Networks | |
|--|---|
| Description | A web based on-line demo of the source code |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#historical-document-line-detection-using-neural-networks-manuscript |

| Electrical Resistivity Tomography: 3DINV | |
|---|---|
| Description | 3DINV User Manual |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#electrical-resistivity-tomography-3dinv |

| CH-CBIR: Content-Based Image Retrieval and Classification in Cultural Heritage Applications | |
|--|---|
| Description | Usage of CNN in CH-CBIR. The Material provides an article as well as a presentation. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#content-based-image-retrieval-and-classification-in-cultural-heritage-applications-ch-cbir |

| VirMuf: Virtual Museum Framework | |
|---|---|
| Description | General Training Material related to the application such as, Manual, introduction to Photography and Photogrammetry etc. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#virtual-museum-framework-virmuf |

| MEDICI and Digital Repositories for CH page | |
|--|---|
| Description | A Presentation on the usage of MEDICI in Digital Cultural Heritage |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#medici-and-digital-repositories-for-ch-page |

| Drupal for Researchers | |
|-------------------------------|---|
| Description | Class that introduces DCH users to Drupal through building their own site. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#drupal-for-researchers |

| Omeka training material | |
|--------------------------------|---|
| Description | A content management system designed for the display of library, museum, archives, and scholarly collections and exhibitions. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#omeka-training-material |

| DSpace training material | |
|---------------------------------|---|
| Description | Introduction to DSpaces. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#dspace-training-material |

| Fedora Commons training material | |
|---|---|
| Description | Introduction to Fedora (F lexible E xtensible D igital O bject R epository A rchitecture). |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#fedora-commons-training-material |

| Koha training material | |
|-------------------------------|---|
| Description | Introduction to Koha Open Source ILS. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#koha-training-material |

| OpenNumisma training material | |
|--------------------------------------|--|
| Description | The platform provides an innovative merge of digital imaging and data management systems that offer great new opportunities for research and the dissemination of knowledge. |

| | |
|----------|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#openumisma-training-material |
|----------|---|

Reconstructing ancient landscapes

| | |
|-------------|---|
| Description | Guidelines on the reconstruction of ancient landscapes. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#ancient-landscape-reconstruction |

Rethinking access to digital information

| | |
|-------------|---|
| Description | Introduction to the idea of Digitalization. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#rethinking-access-to-digital-information |

D3.js for Data Visualization

| | |
|-------------|---|
| Description | Data visualization library. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#d3-js-for-data-visualization |

3.2.3. Life Sciences scientific community

The Life Sciences Scientific Community currently provides the following training material:

Membrane protein tutorial with GROMACS

| | |
|-------------|---|
| Description | A series of steps to set up and run an MD simulation of a membrane protein embedded in a solvated lipid bilayer using the GROMACS program and its associated tools. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#membrane-protein-tutorial-with-gromacs |

| Molecular Dynamics Simulations of BPTI in Vacuum | |
|---|---|
| Description | An overview of classical Molecular Dynamics (MD) simulations and Normal Mode Analysis (NMA) by examining the protein called bovine pancreatic trypsin inhibitor (BPTI) within the framework of the CHARMM program. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#molecular-dynamics-simulations-of-bpti-in-vacuum |

| Molecular Dynamics simulations of lysozyme in water | |
|--|---|
| Description | An overview of classical Molecular Dynamics (MD) simulations and Normal Mode Analysis (NMA) by examining the protein Lysozyme within the frame work of the NAMD program. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#molecular-dynamics-simulations-of-lysozyme-in-water |

| Simulation of a coarse grained DNA molecule in explicit solvent | |
|--|---|
| Description | Tutorial for the simulation of a coarse grained DNA molecule in explicit solvent. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#tutorial-1-simulation-of-a-coarse-grained-dna-molecule-in-explicit-solvent |

| Hybrid solvation: plugging sirah solvent to your atomistic system | |
|--|---|
| Description | Tutorial on Hybrid solvation which demonstrates how to apply the hybrid solvation approach of SIRAH forcefield to speed up the simulation of an atomistic solute. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#tutorial-2-hybrid-solvation-plugging-sirah-solvent-to-your-atomistic-system |

| Simulation of coarse grained proteins in explicit solvent | |
|--|---|
| Description | This tutorial shows how to use the SIRAH forcefield to perform a coarse grained (CG) simulation of a protein in explicit solvent. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#tutorial-3-simulation-of-coarse-grained-proteins-in-explicit-solvent |

| Out of the box simulations of closed circular DNA | |
|--|---|
| Description | This tutorial shows how to use the SIRAH forcefield to perform a coarse grained (CG) simulation of a closed circular DNA in explicit solvent. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#tutorial-4-out-of-the-box-simulations-of-closed-circular-dna |

| PSOMI Workflow | |
|-----------------------|---|
| Description | This workflow contains steps for analysis interaction between small ligand and protein by using ChemSketch, Open Babel, PRODRG and Gromacs on HPC cluster. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#protein-small-organic-molecules-interaction-psomi |

| THEROMGENOME: Execution of Perl Script | |
|---|---|
| Description | User manual for calculating the thermodynamic stability (ΔG) of RNA/DNA duplexes, DNA/DNA duplexes and the difference between DNA/DNA and RNA/DNA duplexes (DNA/DNA – RNA/DNA) by thermogenome.pl. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#thermodynamic-stability-of-dna-dna-and-rna-dna-duplexes-of-entire-genomes-of-eukaryotic-organisms-thermogenome |

| CNCADD: Calculating the local mode frequencies | |
|---|---|
| Description | Calculation of local mode frequencies from classical or ab initio molecular dynamics simulations. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#conventional-vs-novel-computer-assisted-drug-delivery-cncadd |

| Next Generation Sequencing Pipeline: NGS1 | |
|--|---|
| Description | Guidelines for Next generation sequencing of human samples using Illumina NextSeq500 platform. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#next-generation-sequencing-pipeline-ngs1 |

| Classification of Cancer Cells | |
|---------------------------------------|---|
| Description | Guidelines on how to use the CCC application. |
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#classification-of-cancer-cells-ccc |

3.3. Regional community datasets

Below we list the training material available for each scientific community in regards to the VI-SEEM regional community dataset service. The material concerns datasets of regional importance for the scientific communities of interest.

3.3.1. Climate scientific community

The Climate Scientific Community currently provides the following training material:

| Regional Climate Modeling – WRF RCM MENA - CORDEX | |
|--|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#regional-climate-modelling-middle-east-north-africa-wrf-rcm-mena-cordex |

| NetCDF data format user page | |
|-------------------------------------|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools#network-common-data-form-netcdf-data-format-user-page |

3.3.2. Digital Cultural Heritage scientific community

The Digital Cultural Heritage Scientific Community currently provides the following training material:

| Introduction to metadata for digital resources | |
|---|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#introduction-to-metadata-for-digital-resources-2d-3d-page |

| Content aggregation: Tools & guidelines | |
|--|---|
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#content-aggregation-tools-guidelines |

| Selection criteria for the monographic documents in the Banatic collection | |
|---|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#vi-seem-applications |

| Manuscript demo: Historical Document Line Detection Using Neural Networks (A description of the database with handwritten Arabic script) | |
|---|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#historical-document-line-detection-using-neural-networks-manuscript |

| VirMuf: Virtual museum application development (3D models) | |
|---|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#virtual-museum-framework-virmuf |

| RIVEEL3D: Real-time Immersive 3D Virtual Environment for Education and Learning application development (3D model) | |
|---|---|
| Material | https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#real-time-interactive-3d-virtual-environment-for-education-and-learning-riveel3d |

3.4. Application-level services for regional communities

Below we list the training material available for each scientific community in regards to the VI-SEEM Application level services for the regional communities. The material concerns Web-based or visualization services providing easy access to underlying workflows, applications, and resources.

3.4.1. Live Access Server (Climate)

The VI-SEEM Climate Scientific community has provided a detailed user page for the LAS service. The user page walks the user through the features of the LAS service and explains the process for selecting, visualizing and getting access to the available datasets. The user page is available at <https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/climate-software-and-tools>.

3.4.2. *Clowder (Digital Cultural Heritage)*

The VI-SEEM Digital Cultural Heritage scientific community has provided training material on the use of the Clowder service. The material explains in detail the architecture and main idea behind the research data management system and also instructs the user on how to upload new or use the available data collections. The following material is available for Clowder:

- Using the VI-SEEM Clowder Platform (video and presentation) <https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools>
- Medici and digital repositories for Cultural Heritage <https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/digital-cultural-heritage-software-and-tools#medici-and-digital-repositories-for-ch-page>

3.4.3. *ChemBioServer (Life Sciences)*

The VI-SEEM Life Sciences scientific community has provided training material for the use of the ChemBioServer Service. The material provides to the user general recommendation on the use of the service along with a set of step-by-step examples illustrating the functionality provided by ChemBioServer. The material is available in the form of two tutorials. One in an article like format and one in a presentation like format. Both can be found at

<https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#chembioserver>

3.4.4. *AFMM (Life Sciences)*

The VI-SEEM Life Sciences scientific community has provided training material for the use of the AFMM Service. The material provides to the user general recommendation on the use of the service along with a set of step-by-step examples illustrating the functionality provided by AFMM. The material is available in the form of a tutorial and can be found at

<https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#afmm>

3.4.5. *NANO-Crystal (Life Sciences)*

The VI-SEEM Life Sciences scientific community has provided training material for the use of the NANO-Crystal Service. The material provides to the user the associated theoretical background as well as general recommendation on the use of the service along with a set of step-by-step examples illustrating its functionality and capability. The material is available in the form of a tutorial and can be found at

<https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#nano-crystal>

3.4.6. Subtract (Life Sciences)

The VI-SEEM Life Sciences scientific community has provided training material for the use of the Subtract Service. The material provides a short tutorial on the general idea behind the use of the Subtract Service and an example demonstrating its capabilities. The tutorial can be found in:

<https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#subtract>

3.4.7. DICOM Network (Life Sciences)

The VI-SEEM Life Sciences scientific community has provided training material for the use of the DICOM Network Service. The material provides to the user a presentation on how a researcher can use the Service. The material is available at

<https://training.vi-seem.eu/index.php/domain-specific-software-and-tools/life-science-software-and-tools#visualization-medical-image-processing-dicom-network-dicom>

3.5. Scientific visualization

Scientific visualization is an interdisciplinary branch of science primarily concerned with the visualization of three-dimensional phenomena (architectural, meteorological, medical, biological, etc.), where the emphasis is on realistic renderings of volumes, surfaces, illumination sources, and so forth, perhaps with a dynamic (time) component. Scientific visualization provides the following training material targeting all Scientific Communities. This section of the training material is organized in three different sections (tabs), namely General Training Material, Climate and Digital Cultural Heritage. Below we provide the corresponding material:

3.5.1. General training material

| Large data visualization | |
|--------------------------|---|
| Description | Introduction to the concepts of visualization with a focus on parallel computing to handle large datasets. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#large-data-visualization |

| Paraview | |
|-------------|---|
| Description | By example introduction to the use of the Paraview visualization tools. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#paraview |

| D3.js for Data Visualization | |
|-------------------------------------|---|
| Description | Data visualization library. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#d3-js-for-data-visualization |

3.5.2. Climate

| NCAR graphics user page | |
|--------------------------------|---|
| Description | NCAR Graphics is a Fortran and C based software package for scientific visualization. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#ncar-graphics |

| NCL user page | |
|----------------------|---|
| Description | NCL is an interpreted language designed specifically for scientific data analysis and visualization |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#ncar-command-language-ncl |

| VisTrails | |
|------------------|--|
| Description | VisTrails is an open-source scientific workflow and provenance management system that supports data exploration and visualization. The training material provides access to the VisTrails Wiki and an example of a VisTrails Workflow. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#vistrails |

3.5.3. Digital Cultural Heritage

| Landscape Services | |
|---------------------------|---|
| Description | A set of responsive web services that include large terrain datasets generation, 3D landscape composing and 3D model processing, leveraging on powerful open-source frameworks and toolkits such as GDAL, OSGjs, OpenSceneGraph and ownCloud. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#landscape-services |

| Reconstructing ancient landscapes | |
|--|---|
| Description | Guidelines on the reconstruction of ancient landscapes. |

| | |
|----------|---|
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#ancient-landscape-reconstruction |
|----------|---|

| Introduction to Stereoscopy for Archaeology | |
|--|---|
| Description | Introduction to techniques for recording three-dimensional visual information by using the characteristics of human binocular vision to recreate the illusion of depth of an image as of the real world. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#introduction-to-stereoscopy-for-archaeology |

| RTI Imaging, PTM Dome and 360 degree imaging of Cylindrical Surfaces | |
|---|---|
| Description | Introduction to Reflection Transformation Imaging. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/scientific-visualisation#rti-imaging-ptm-dome-and-360-degree-imaging-of-cylindrical-surfaces |

4. User documentation and training material for VI-SEEM VRE contributors

In this section we list the training material for user community users that want to contribute their services, modules, codes, workflows and datasets to the VI-SEEM Virtual Research Environment. First we provide the specific tutorials designed by the VI-SEEM community for uploading the contribution to the related services. Then we provide a set of guidelines for integrating the contribution to the VRE making it available and usable through the VRE portal.

4.1. *Uploading information to VI-SEEM services*

4.1.1. *VI-SEEM service catalogue/portfolio*

Community users that want to list their services through VI-SEEM Virtual Research Environment should first register their service at the VI-SEEM service catalog. A detailed guide for this process is provided at https://wiki.vi-seem.eu/index.php/VI-SEEM_Service_catalog_service_enablers_guide. The guide gives step-by-step directions to the interested user on how to log-in, create and populate a new service with the required information.

4.1.2. *VI-SEEM code repository*

Community users that want to list and share their code through the VI-SEEM Virtual Research Environment should first upload their code to the code repository. At the Project wiki page located at

http://wiki.vi-seem.eu/index.php/Source_Code_Repository there is a very detailed how-to document. This document covers both Web based and command line based access to the repository. There are detailed instructions on how to obtain access to the repository system, how to set up ssh keys, how to work with projects, instructions on pulling, adding, committing and pushing changes as well as a section on configuring git on a local machine. The document contains many screen-shots of the web user interface and code examples for all important parts of the repository service.

4.1.3. *VI-SEEM repository*

Community users that want to share their datasets, articles, audiovisual material, digital library collection and more can do so by uploading them to the VI-SEEM repository. A detailed tutorial explaining the repository organization, data collections per community and step-by-step instructions on how to register and upload material is available through the VI-SEEM training portal at <https://training.vi-seem.eu/index.php/data-and-visualizations/storage-services>.

4.1.4. Support ticket system

A user manual for the Support Ticket System is located at https://wiki.vi-seem.eu/index.php/Support_Ticket_System. This manual covers both end-user as well as agent use of the system. Introduction documents basic concepts and explains the basic work-flow and ticket life-cycle. End user documentation guides users through basic setup and access to the system and working with the support tickets. User guide for agents describes working with users and working with tickets. The manual is complemented by screen-shots of every described action.

4.2. Guidelines for uploading information for VI-SEEM domain specific services

To ensure that all relevant information is uploaded to the VI-SEEM services, we prepared a set of guidelines for each of the community-developed service modules and services. These guidelines assist the developers for uploading all relevant information for their applications. Upon completion of the guidelines the Scientific Community Leader is notified in order to perform quality check and verification of the material. These steps should be followed when listing code or datasets to the VRE portal. The guidelines for each of the domain specific service are available in the VRE portal under the "How to contribute" section for each service.

4.2.1. VI-SEEM scientific application environment guidelines

Adding an application or service module to the scientific application environment is done following these guidelines. The responsible scientist needs to register the service module on the Vi-SEEM service registry and upload relevant code in the Vi-SEEM code repository. The responsible scientist will then make sure that each service module, as defined in the VRE integration plan, is set up correctly, and that it works and is accessible to users as expected. The documentation must be made available in the Vi-SEEM wiki, and must entail instructions on how to access, compile and/or use each service module. The training material will cover scientific aspects of the application, and must be hosted on the Vi-SEEM training portal. Any datasets necessary for the usage of the service module will be uploaded on the Vi-SEEM dataset repository. Upon completion of the aforementioned steps, the Scientific Community Leader is notified to perform the quality check and verification of the material. The detailed guidelines for contributing to the Scientific Application Environment service are located in the VRE portal at <https://vre.vi-seem.eu/index.php/scientific-application-environment/how-to-contribute>.

4.2.2. Workflow and software repository tools

Workflow, pipeline and software repository tools should be added to the VRE portal through the following guidelines. First, the responsible scientist will register the workflow, pipeline or software repository tool on the Vi-SEEM service registry and upload the relevant content on the Vi-SEEM code or dataset repository, depending on

the content to be uploaded. Documentation on how to access, set up and use the tools will be uploaded on the Vi-SEEM wiki, while training material will be hosted on the Vi-SEEM training portal. Following the completion of the guidelines, the Scientific Community Leader will perform the quality check and verification of the tools for the final approval. The detailed guidelines for contributing to the Workflow, pipeline and software repository tools service are located in the VRE portal at <https://vre.vi-seem.eu/index.php/workflow-pipeline-and-software-tools-repository/how-to-contribute>.

4.2.3. Regional community datasets

To add regional community datasets on the VRE portal, the responsible scientist needs to follow these guidelines. The datasets will need to be registered on the Vi-SEEM service registry, and uploaded on the Vi-SEEM dataset repository, VI-SEEM application specific services or linked through an external source. The description of the datasets, along with information on the conditions the data were generated or acquired and contact details of the responsible scientist will be uploaded on the Vi-SEEM wiki. The Scientific Community Leader will perform a quality check and verification of the datasets to ensure that they comply with regulations and all relevant content is present, as described. The detailed guidelines for contributing to the Regional community datasets service are located in the VRE portal at <https://vre.vi-seem.eu/index.php/regional-community-datasets/how-to-contribute>.

4.2.4. Application-level services for the regional communities

Current application-level services, such Clowder, LAS, ChemBioServer, AFMM, NANO-Crystal, Subtract and DICOM cover a multitude of applications in Cultural Heritage, Climate Sciences and Life Sciences, respectively. Potential additional application-level services can be added to enhance the scope of Vi-SEEM, following these guidelines. The service should be registered by the responsible scientist on the Vi-SEEM service registry, while a description will be uploaded on the Vi-SEEM VRE-Portal. Documentation and training material will be uploaded on the Vi-SEEM training portal. For application-level services, the Scientific Community Leader is responsible for the quality check and verification that all material is adequately presented and can be accessed by the Vi-SEEM collaborators. The detailed guidelines for adding a new Application-level service are located in the VRE portal at <https://vre.vi-seem.eu/index.php/application-level-services-for-the-regional-communities/how-to-contribute>.

5. User documentation and training material for generic VRE services

5.1. VI-SEEM e-infrastructure services

5.1.1. HPC

VI-SEEM training material related to High Performance Computing (HPC) is available at <https://training.vi-seem.eu/index.php/common-computing-resources/hpc>. This section of the VI-SEEM training portal covers all relevant topics needed for VI-SEEM developers so that they can efficiently use HPC infrastructure. As outlined in Section 2.2.2, HPC training material is organized in four sections: "Practical HPC", "Development", "Improvement" and "Applications".

Section "Practical HPC" provides different training topics relevant for usage of HPC systems. Less experienced users can learn about the foundations of supercomputing, basic Linux commands, and usage of HPC clusters in the "Supercomputing Basics" tab. Once they start using HPC resources in a more serious manner, within the subsections "Scripting" and "Version Control", users can find useful information about various scripting languages and techniques that will help them automate tasks (e.g. submitting jobs, more efficient analysis of obtained results), as well as show them how to use version control software, namely git, in the development cycle of their own code. The training material appearing in "Practical HPC" has the following structure:

- Super Computer Basics
 - Module Framework
 - Workshop of Clouds, Cluster and High Performance Computing Infrastructures
 - Introduction to Linux/Linux shell – 1
 - Introduction to a Linux Shell – 2
- Scripting
 - Python
 - Automated Builds
 - Balancing Scripts and Combined Code
- Version Control
 - Git-Introduction
 - Git-Collaboration
- Parallel Tools Platform
 - PTP – Installation
 - PTP – Usage
 - PTP – debugging

Different topics relevant for development of user's application are covered in section "Development". It provides introductory materials for C, C++, and Fortran programming languages, and more advanced material for the increasingly popular Python programming language. For development of parallel applications users can

visit "MPI" and "OpenMP" subsections which provide a large amount of available training material for these two parallel programming paradigms. For programming general-purpose graphics processing units (GPGPUs) that are available on some VI-SEEM HPC resources, subsection "GPU Programming" provides related training materials. Links to content created and gathered during HP-SEE project, dedicated to HPC applications development, are also available within this section. The structure of the training material on "Development" is the following:

- Programming
 - Introduction to C++
 - Introduction to C
 - Introduction to Fortran
- Python
 - Introduction to Python – Part 1
 - Introduction to Python – Part 2
 - Python Unit Testing
 - Python for High Performance
- OpenMP
 - OpenMP
 - Introduction to share memory parallel programming with OpenMP
 - Online Introduction to OpenMP
 - Introduction to OpenMP
 - OpenMP optimization
 - Advanced OpenMP – Part 1
 - Advanced OpenMP – Part 2
 - Compiler Directives for Accelerators - 1
 - Compiler Directives for Accelerators - 2
 - Compiler Directives for Accelerators - 3
- MPI
 - Programming with MPI
 - Programming with MPI & OpenMP
 - Message Passing Interface (MPI) Basics
 - Introduction to parallel computing concepts and techniques
 - MPI
 - Introduction to Parallel programming with MPI
 - MPI point-to-point
 - MPI collective communications
 - MPI one-sided communication
 - MPI advanced topics
- GPU Programming
 - HPCReS 2014 – Workshop on HPC research services (GPU Tutorial)
 - Introduction to GPU computing
- General Training Material
 - Parallel Computing Course
 - HPC training techniques
 - HP-SEE Training Center

For improving and debugging of developed code so that it can efficiently run on relatively complex and often heterogonous HPC resources, section "Improvement" through its subsections provides links to training material related to code performance analysis, optimization, porting and debugging techniques, and covers a significant number of different software tools used for these purposes. The training material in Improvement has the following structure:

- Performance Analysis
 - Introduction to Performance Analysis
 - Score-P Part 1
 - Score-P Part 2
 - Cube
 - ParaProf
 - Scalasca
 - Vampir
 - Periscope
 - Performance Analysis – Conclusions
- Code Improvement and Debugging
 - Optimization techniques for scalability
 - Advanced Application Porting and Optimization
 - Profiling and Debugging
 - Optimization and Scalability
 - DDT Debugger

"Applications" section of HPC training materials in VI-SEEM Training Portal provides material related to different practical applications of HPC where users can see how HPC resources are used in solving of specific problems.

5.1.2.Cloud

VI-SEEM Training material related to Cloud computing is available at <https://training.vi-seem.eu/index.php/common-computing-resources/cloud>. This section provides information about general concepts of Cloud. Namely this provides a link to the webpage of the course on Cloud Computing taught by Dana Petcu:

<https://users.info.uvt.ro/~petcu/cloud.html>.

General information cover Cloud enabling technologies and its main service models: infrastructure as a service (IaaS), platform as a service (PaaS), and software as a service (SaaS).

Training material related to usage of Cloud resources contains descriptions and guides to specific Cloud environments available in VI-SEEM e-Infrastructure, like Openstack. This practical material shows users how to use available Cloud resources in production for their applications.

Information related to various Cloud based applications like Big Data applications, e-government tools, or digital preservation projects are also available in Cloud section of VI-SEEM Training Portal.

5.1.3. Grid

VI-SEEM training material related to Grid computing can be found at <https://training.vi-seem.eu/index.php/common-computing-resources/grid>. This page gives overview of Grid computing in general and provides all necessary information needed for efficient usage of Grid resources provided within the VI-SEEM project. Users are provided information on how to setup accounts on Grid User Interface, manage X.509 certificates, join Virtual Organizations, submit different types of Grid jobs to the infrastructure and retrieve results, and manage data on Grid storage resources. In addition to various presentations, full step-by-step examples with necessary commands and JDL code are provided.

In addition to material for users, Grid section of VI-SEEM Training Portal also provides material useful to Grid resource centers administrators which contains detailed information about installation of various types of Grid services.

The training portal page which provides general training material is organized in the five following sliders

| Workshop on Grid Training for Power Users | |
|--|--|
| Description | <p>It provides a link to the webpage of the training material presented in the workshop "Grid Training for Power Users" held at the IPB in Serbia, on May 28, 2012. It provides hands-on training for Grid users covering the topics described below</p> <ul style="list-style-type: none"> • Setting Up User Account • Single Job Submission • Job Collections Submission • Parametric Job Submission • Direct Acyclic Graphs (DAG) Job Submission • Message Passing Interface (MPI) Job Submission • Data Management • Advanced Job Submission |
| Material | <p>https://training.vi-seem.eu/index.php/common-computing-resources/grid#workshop-on-grid-training-for-power-users</p> |

| Workshop "EGI HandsOn Training for AEGIS Site Administrators" | |
|--|---|
| Description | <p>This provides a link to the webpage of the training material presented in the workshop "EGI HandsOn Training for AEGIS Site Administrators" held at the IPB in Serbia, on November 23, 2012, This provides hands-on training for Grid site administrators covering topics such as:</p> <ul style="list-style-type: none"> • Grid Operations tools and procedures • Grid site installation • Operating system installation • CREAM CE and site BDII installation • Worker node (WN) installation |

| | |
|----------|---|
| | <ul style="list-style-type: none"> Storage Element (SE) installation |
| Material | https://training.vi-seem.eu/index.php/common-computing-resources/grid#workshop-egi-hands-on-training-for-aegis-site-administrators |

Workshop "EGI Hands On Training for AEGIS Users"

| | |
|-------------|---|
| Description | <p>This provides a link to the webpage of the training material presented in the workshop "EGI HandsOn Training for AEGIS Users" held at the IPB in Serbia, on March 25, 2011. This provides hands-on training for Grid site administrators covering topics such as:</p> <ul style="list-style-type: none"> Linux shell environment Setting up the user account gLite workload management Single job submission Parametric job submission Data Management |
| Material | https://training.vi-seem.eu/index.php/common-computing-resources/grid#workshop-egi-hands-on-training-for-aegis-users |

Workshop "EGI Training for AEGIS Site Administrators"

| | |
|-------------|--|
| Description | <p>This provides a link to the webpage of the training material presented in the workshop "EGI Training for AEGIS Site Administrators" held at the IPB in Serbia, on March 7, 2011, This provides hands-on training for AEGIS site administrators covering topics such as:</p> <ul style="list-style-type: none"> Grid Operations tools and procedures AEGIS Operations and Monitoring tools AEGIS Centralized APEL service Standard Grid site installation User Interface (UI) CREAM CE and site BDII Worker node (WN) Storage Element (SE) |
| Material | https://training.vi-seem.eu/index.php/common-computing-resources/grid#workshop-on-egi-training-for-aegis-site-administrators |

Grid Examples Page

| | |
|-------------|---|
| Description | This page contains various examples how to submit jobs on the Grid as well as basic storage resources interaction tutorial. Examples are committed to new users, and people who want to try EGI Grid. |
| Material | https://training.vi-seem.eu/index.php/common-computing-resources/grid#grid-examples-page |

5.2. Event-related training materials

In the training portal, at the header once you move the cursor over the button Event Related Training Materials, a drop down window appears which lists all the VI-SEEM training events which have taken place to date. In addition by clicking on the button "Event Related Training Material" the user is directed to the webpage: <https://training.vi-seem.eu/index.php/event-related-material> which lists all the past VI-SEEM training events. The entries direct the user to the webpage of each training event which presents the time schedule and provides links to all the presentations in .pdf format. Therefore the user can read the actual presentations. In some special cases such as the "PRACE 2017 Spring School joint event with VI-SEEM" the webpage provides links to the actual presentations in YouTube.

Training events are identified with an acronym. The first part of the acronym identifies the Project which organizes the event; hence, for VI-SEEM all events begin with "VI-SEEM" with the only exception "PRACE 2017 Spring School joint event with VI-SEEM" which was organized in co-operation with PRACE. The next part of the acronym identifies whether the training is National (NAT) or Regional (REG). The third part of the acronym indicates the partner holding the event (if NAT) and the last piece of the acronym recalls the Scientific Community.

The following table presents the training events in chronological order. This is also the way the training events appear in the training portal.

| Acronym | Date/Place | Title/link |
|-------------------------|---|---|
| VI-SEEM NAT-MD LS | April 22, 2016 Chişinău, Moldova | Characteristics, technical parameters and special features of distributed informational system «DICOM Network» |
| | | http://events.hpc.grnet.gr/event/15/timetable/#20160422 |
| VI-SEEM REG LS+CL+CH | June 24, 2016, Belgrade, Serbia | Introduction to Hadoop |
| | | http://events.hpc.grnet.gr/event/19/timetable/#20160624 |
| VI-SEEM NAT-BG LS+CL+CH | July 7, 2016, Sofia, Bulgaria | Introduction in Parallel Programming and Optimization for Intel Xeon Phi Architecture |
| | | http://events.hpc.grnet.gr/event/20/timetable/#20160707 |
| VI-SEEM NAT-MD LS | July 13, 2016, Athens, Greece | National Dissemination Event with support of AITT – "DICOM Network" |
| | | http://events.hpc.grnet.gr/event/21/ |
| VI-SEEM NAT-MK LS+CL | August 30, 2016, Skopje, FYR of Macedonia | Life sciences and Climate national training event |
| | | http://events.hpc.grnet.gr/event/22/other-view?view=standard |
| VI-SEEM REG LS | October 19-21, 2016, Belgrade, Serbia | VI-SEEM e-Infrastructure services, Molecular Dynamics Simulations of Biomolecules and Computer-Aided Drug Design |

| | | |
|-----------------------|---|---|
| | | http://events.hpc.grnet.gr/event/23/other-view?view=standard |
| VI-SEEM NAT-GE CL | October 29, 2016, Tbilisi, Georgia | Climate national training event http://events.hpc.grnet.gr/event/27/timetable/#20161029 |
| GRNET event | November 9 2016, Athens, Greece | Biomolecular modelling training on National HPC Infrastructure ARIS, November http://events.hpc.grnet.gr/event/31/ |
| GRNET event | December 19 2016, Athens, Greece | Meteorological and Climate Modelling using WRF http://events.hpc.grnet.gr/event/35/ |
| VI-SEEM NAT-EG CH | February, 6-8, 2017, Alexandria, Egypt | Digital cultural heritage training event at BA http://events.hpc.grnet.gr/event/36/other-view?view=standard |
| VI-SEEM NAT-AL CL | April 13, 2017, Tirana, Albania | VI-SEEM National Dissemination and Training Event https://events.hpc.grnet.gr/event/45/material/0/0.pdf |
| PRACE & VI-SEEM event | April 25-27, 2017, Nicosia, Cyprus | PRACE 2017 Spring School joint event with VI-SEEM https://events.prace-ri.eu/event/601/timetable/#20170425 |
| VI-SEEM NAT-IL CL | June 4, 2017, Tel-Aviv, Israel | Introduction to Google Earth Engine (GEE) and Remote Sensing and Climate Applications link:http://events.hpc.grnet.gr/event/47/other-view?view=standard |
| VI-SEEM REG CL | (Upcoming event) October 11-13, 2017 | Regional Climate training event http://events.hpc.grnet.gr/event/50/other-view?view=standard |

5.3. Training material on data

The VI-SEEM Training Portal provides material on topics related to data, such as data management tools, metadata and data formats used in particular Scientific Disciplinaries such as the NETCDF used in the Climate Scientific Community. The training portal page dedicated to Data can be accessed through the link: <https://training.vi-seem.eu/index.php/data-and-visualizations/data#dspace-training-material>. This page is organized in 3 sections (tabs), namely in 1. General Training Material, 2. Climate and 3. Digital Cultural Heritage. The training material which is available is the following:

5.3.1. General training material

| Hadoop | |
|---------------|---|
| Description | This provides general material on several aspects of Hadoop such as: <ul style="list-style-type: none"> • A Brief Overview of Hadoop • Access to IPB Hadoop Cluster • Hadoop MapReduce • Hadoop MapReduce Streaming • Twitter user ranking • Hands on: Vi-SEEM Introduction to Hadoop |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#hadoop |

| DSpace training material | |
|---------------------------------|---|
| Description | Introduction to DSpaces. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#dspace-training-material |

5.3.2. Climate

| Network Common Data Form: NetCDF data format user page | |
|---|---|
| Description | The training material on NetCDF provides access to the NetCDF user page where one can find documentation and support on issues on NetCDF. |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#network-common-data-form-netcdf-data-format-user-page |

5.3.3. Digital Cultural Heritage

| Introduction to Metadata for Digital Resources (2D/3D) page | |
|--|---|
| Description | Basic Introduction to metadata in Digital Cultural Heritage |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#introduction-to-metadata-for-digital-resources-2d-3d-page |

| Content aggregation: Tools & guidelines | |
|--|---|
| Description | Guidelines on the use of the Linked Heritage Aggregator (MINT) |
| Material | https://training.vi-seem.eu/index.php/data-and-visualizations/data#content-aggregation-tools-guidelines |

5.4. VI-SEEM storage and data services

The VI-SEEM Storage Services provide different type of basic data storage possibilities for the users of the VREs. The training material for the VI-SEEM data Storage Services is available at https://wiki.vi-seem.eu/index.php/Generic_Data_Services_Training.

The training material provides information about the VI-SEEM Simple Storage Service (VSS), the VI-SEEM Repository Service (VRS) and the VI-SEEM Archival Service (VAS). The training material describes the services in detail, it shows the way how the users can access and use them, and it also contains description of the typical use cases and best practices of the specific services.

The VI-SEEM Data Services are supplementary services to the generic data services. Using the Data Services the VRE users can perform high level, sophisticated data discovery and data analysis tasks on the data stored in the different VI-SEEM Storage Services. The training material for the VI-SEEM Data Services is available at https://wiki.vi-seem.eu/index.php/Generic_Data_Services_Training.

The training material provides information about the VI-SEEM Data Discovery Service (VDDS) and the VI-SEEM Data Analysis Service (VDAS). The training material describes the services the way how the users can access and use them, and it also presents the use cases and best practices associated with these services.

6. Conclusions

This document provided an overview of the user-oriented documentation and training material for the VRE services. WP5 oversees the integration of software tools, workflows, datasets and application-specific services to the VRE. As part of this it collects and lists, through the VRE portal, any available material that will assist the user communities of developing and integrating their application and use cases in the VRE.

The deliverable provides the material made available through the 1st, 2nd and 3rd Integration Phases. The 1st integration Phase was completed at the end of M12 of the project and the 2nd integration phase was completed at the end of M18. The 3rd Integration phase is still on going and is expected to end by M26. By that time all the training material is expected to be uploaded. The documentation and training material provided by the use cases along the integration phases is now available to the Scientific Communities in order to be able to use the tools and datasets made available. Furthermore, documentation and training material will be made available as the current integration phase progresses.

The deliverable also provides documentation for contributing to the VRE environment. Users of the VRE that want to make available their software, datasets and services through the VRE are given specific guidelines how to do so and what material they should be made available.

Finally, documentation and training material for the use of the VI-SEEM generic services, deployed by WP3 and WP4, is also available to both user categories via the VI-SEEM training portal and the VI-SEEM VRE portal.

User-oriented documentation and training material is constantly updated as new services are being integrated into the VI-SEEM VRE.

Deliverable D5.3 is now incorporating the comments given by the reviewers as a result of the 1st periodic review. It describes improved access and presentation of the training material. A number of changes and updates have been made. The consortium has kept the high-level organization of the front page and at the same time reorganized each section in meaningful categories captured by different tabs. These categories were chosen according to practical criteria, depending on the scientific community, so that they provide more intuitive, quick and direct access to the relevant training material. These sub-sections are subsequently organized in different parts directing the user to the relevant training material.